

- **SANS Model Function Documentation**

v4.00

FEB 2008 SRK

This help file contains a listing of all of the model functions currently available in the NIST SANS analysis package. Now there should be no excuse for anyone not reading the documentation since the model documentation is linked to each model through the [SANS Model Picker](#). Documentation for each model includes the details of what is calculated, its use, a schematic of the structure (if necessary), an example plot, and references.

Each of the model fitting functions is constructed as a Macro:Function pair. The Macro is called by the user (that's you) from the SANS Models menu and sets up the calculation, creates the coefficient table, calls the function, and draws the graph. Then any change in the coefficients is reflected in the model on the graph, which is automatically recalculated. All of the models are written in this way, so they will all behave the same.

Almost all of the models can be plotted and fitted to data after convolution with the instrumental resolution function, which is quite different for SANS and USANS data sets. Resolution corrections should not be ignored during data analysis. The details of [Resolution Smearing](#) can be found by following the link to the end of the SANS Analysis Documentation.

Some models are for interacting particles, where the intensity is a combination of form factor and structure factor effects. For hard spheres, this calculation can be done exactly. For other interaction potentials or anisotropic particles, approximations must be made. For details on how this is done, see the section: [How Form Factors and Structure Factors are Combined](#)

General Instructions for how to perform curve fitting to analyze your SANS data are found in a separate help file, [SANS Data Analysis Documentation](#).

If you use this software to analyze your data, please reference:

"Reduction and Analysis of SANS and USANS Data Using IGOR Pro"  
S. R. Kline, *J. Appl. Cryst.* **39** (2006) 895-900.

## **Model Functions for Scattering**

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See Also: [How Form Factors and Structure Factors are Combined](#)

## [Interacting Particles](#)

These are exact solutions that correctly incorporate hard sphere interactions for populations of hard spheres that are not monodisperse.

[Polydisperse Hard Spheres](#)  
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Many of the form factor models above have been combined with structure factors. These are contained in the procedure files ending in "\_Struct.ipf".

## [Polymer Models](#)

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### • [Form Factors for Simple Shapes](#)

#### [Monodisperse Spheres](#)

##### **MACRO : FUNCTION**

PlotSphereForm() : SphereForm(w,y,x)

Wave extension:     \_sf

File:

[Sphere.ipf](#)

Requires:

GaussUtils.ipf

PlotUtils.ipf

##### **AUTHOR/MODIFICATION**

Steve Kline   06 NOV 1998

##### **APPROVED FOR DISTRIBUTION**

Sungmin Choi 02 FEB 1999

##### **DESCRIPTION**

Calculates the form factor,  $P(q)$ , for a monodisperse spherical particle with uniform scattering length density. The form factor is normalized by the particle volume as described below. Resolution smeared version is also provided.

##### **VARIABLES**

Input Variables (default values):

parameters_sf	coef_sf
scale	1
Radius (Å)	60
SLD sphere (Å <sup>-2</sup> )	1e-06
SLD solvent (Å <sup>-2</sup> )	6.3e-06
bkgd (cm <sup>-1</sup> )	0.01

## USAGE NOTES

The function calculated is:

$$P(q) = \frac{scale}{V} \left[ \frac{3V(\Delta\rho)(\sin(qr) - qr \cos(qr))}{(qr)^3} \right]^2 + bkg$$

The returned value is scaled to units of [cm<sup>-1</sup>]

Scattering contrast ( $\Delta\rho$ ) = SLD (core) - SLD (solvent)

w[0] (scale) and w[2] (contrast) are both multiplicative factors in the model and are perfectly correlated. One or both of these parameters must be held fixed during model fitting.

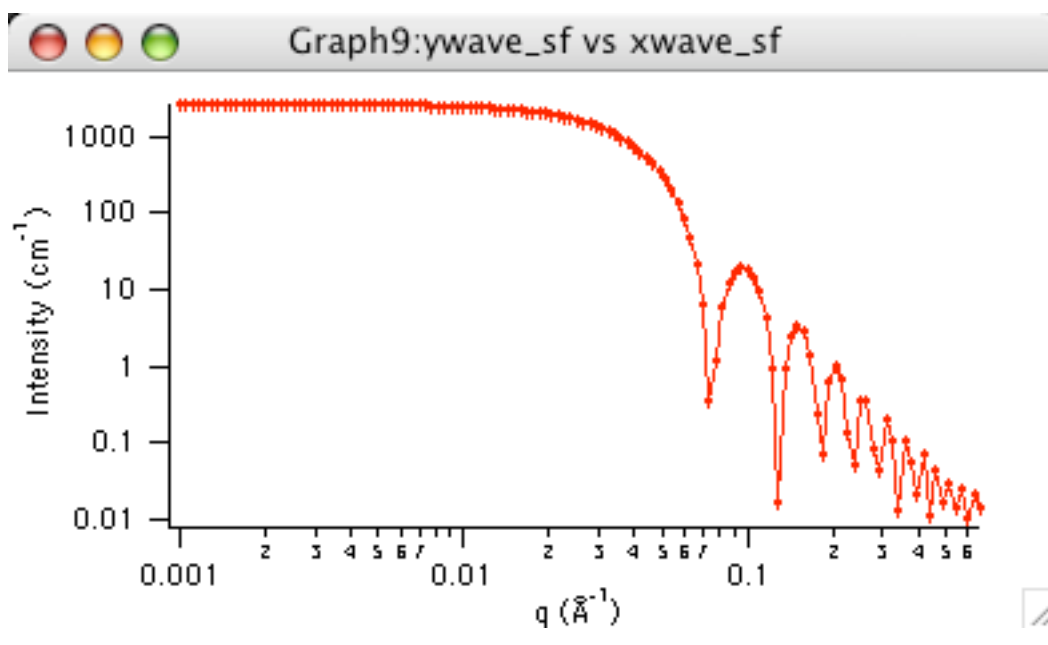
If the scale factor w[0] is set equal to the particle volume fraction,  $\phi$ , then the returned value is the scattered intensity per unit volume,  $I(q) = \phi * P(q)$ . However, no interparticle interference effects are included in this calculation.

## REFERENCE

Guinier, A. and G. Fournet, "Small-Angle Scattering of X-Rays", John Wiley and Sons, New York, (1955).

## TEST DATASET

This example dataset is produced by running the Macro PlotSphereForm(), using 128 data points, qmin = 0.001 Å<sup>-1</sup>, qmax = 0.3 (Å<sup>-1</sup>) and the above default coef\_sf values.



### Core-Shell Spheres

#### **MACRO : FUNCTION**

PlotCoreShellSphere() : CoreShellForm(w,y,x)

Wave extension: \_css

File:

CoreShell.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

#### **AUTHOR/MODIFICATION**

Steve Kline 06 NOV 1998

#### **APPROVED FOR DISTRIBUTION**

Sungmin Choi 02 FEB 1999

#### **DESCRIPTION**

Calculates the form factor,  $P(q)$ , for a monodisperse spherical particle with a core-shell structure. The form factor is normalized by the total particle volume. Resolution smeared version is also provided.

#### **VARIABLES**

Input Variables (default values):

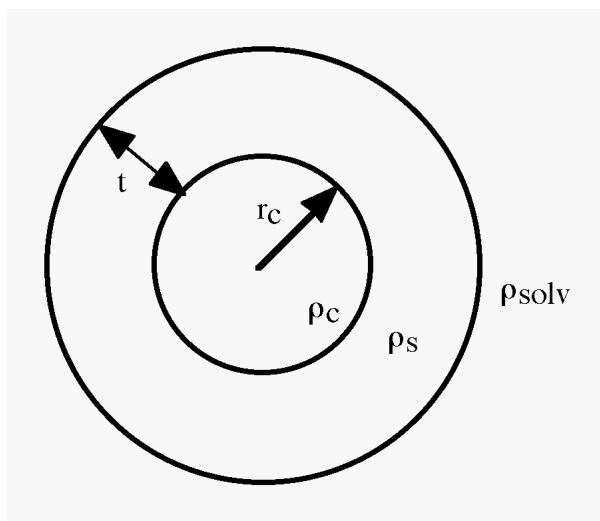
Point	parameters_css	coef_css
0	scale	1
1	core radius (A)	60
2	shell thickness (A)	10
3	Core SLD (A-2)	1e-06
4	Shell SLD (A-2)	2e-06
5	Solvent SLD (A-2)	3e-06
6	bkg (cm-1)	0.001

## USAGE NOTES

The function calculated is:

$$P(q) = \frac{scale}{V_s} \left[ \frac{3V_c(\rho_c - \rho_s)j_1(qr_c)}{qr_c} + \frac{3V_s(\rho_s - \rho_{solv})j_1(qr_s)}{qr_s} \right]^2 + bkg$$

where  $j_1(x) = (\sin x - x \cos x) / x^2$ ,  $r_s = r_c + t$ , and  $V_i = (4\pi/3)r_i^3$ . The returned value is scaled to units of  $[cm^{-1}]$ .



w[0] (scale) and the SLD's are multiplicative factors in the model and are perfectly correlated. No more than one of these parameters can be free during the model fitting.

If the scale factor w[0] is set equal to the particle volume fraction,  $\phi$ , the returned value is the scattered intensity per unit volume,  $I(q) = \phi * P(q)$ . However, no interparticle interference effects are included in this calculation.

Scattering from monodisperse vesicles can be calculated by setting the core SLD equal to the solvent SLD.

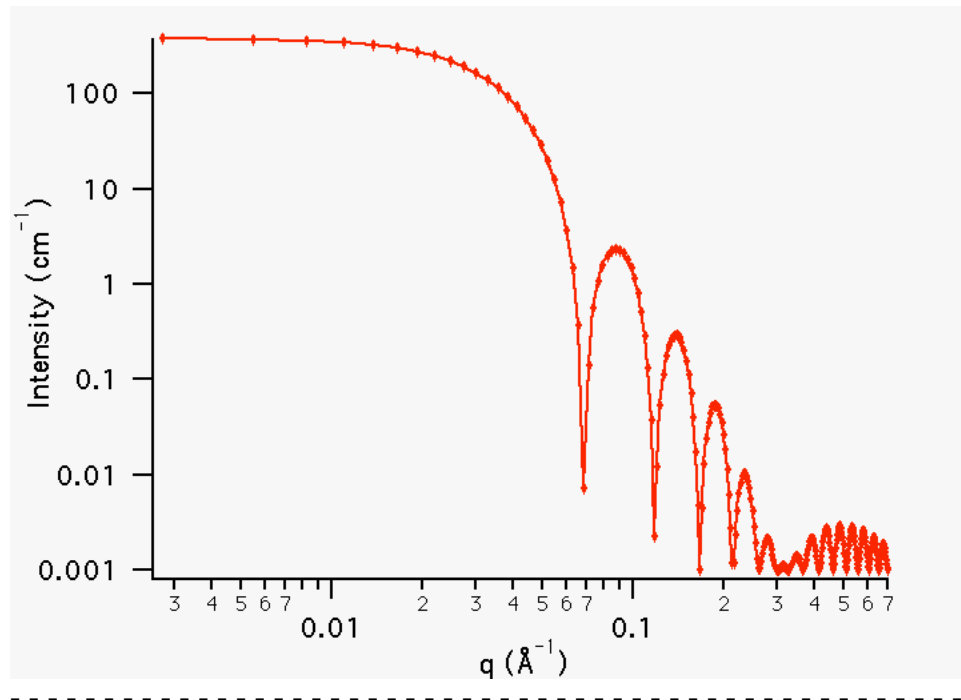
## REFERENCE

Guinier, A. and G. Fournet, "Small-Angle Scattering of X-Rays", John Wiley and Sons,

New York, (1955).

### TEST DATASET

This example dataset is produced by running the Macro PlotCoreShellForm(), using 256 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_css values.



### Unilamellar Vesicles

#### MACRO : FUNCTION

PlotVesicle() : VesicleForm(w,y,x)

Vesicle\_Volume\_N\_Rg()

Wave extension:     \_vesicle

File:

Vesicle\_UL.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

#### AUTHOR/MODIFICATION

Steve Kline   13 JUL 2004

#### APPROVED FOR DISTRIBUTION

Derek Ho      11 AUG 2004

#### DESCRIPTION

Calculates the form factor,  $P(q)$ , for a monodisperse, unilamellar vesicle. The form factor is normalized by the volume of the shell, rather than the total particle volume.

Resolution smeared version is also provided.

## VARIABLES

Input Variables (default values):

Point	parameters_vesicle	coef_vesicle
0	scale	1
1	core radius (A)	100
2	shell thickness (A)	30
3	Core and Solvent SLD (A-2)	6.36e-06
4	Shell SLD (A-2)	5e-07
5	bkg (cm-1)	0

## USAGE NOTES

The function calculated is:

$$I(q) = \frac{scale}{V_{shell}} \left[ \frac{3V_1(\rho_1 - \rho_2) j_1(qR_1)}{qR_1} + \frac{3V_2(\rho_2 - \rho_{solv}) j_1(qR_2)}{qR_2} \right]^2 + bkg$$

where the structure is as shown below, and the following notation applies. The functional form is identical to a "typical" core-shell structure, except that the scattering is normalized by the volume that is contributing to the scattering, namely the volume of the shell alone. Also, the vesicle is best defined in terms of a core radius (=  $R_1$ ) and a shell thickness,  $t$ . Then the radii  $R_1$  and  $R_2$  are defined as:

$$R_1 = R_{core}$$

$$R_2 = R_{core} + t$$

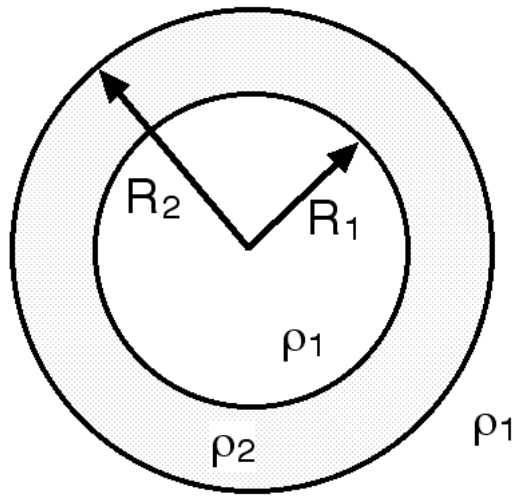
$$V_{shell} = (4\pi/3)[R_2^3 - R_1^3]$$

$$V_i = (4\pi/3)R_i^3$$

and

$$j_1(x) = (\sin x - x \cos x) / x^2$$





With this normalization, if the scale factor is set to be the volume fraction of the "shell" material (for example, the total lipid volume fraction) then the calculated intensity is the macroscopic cross section. This volume fraction is NOT the volume that the vesicles exclude in the solution in the context of excluded volume interactions. Distributing a certain volume fraction of material,  $\phi$ , in identical vesicles with shell volume  $V_{\text{shell}}$ , yields the number density of vesicles,  $n = \phi/V_{\text{shell}}$ . The number density of vesicles is calculated in the macro provided. The volume fraction of solution occupied (excluded) by the vesicles is larger (often much larger!) and is calculated as  $\phi(\text{excluded}) = n \cdot V_{\text{total}}$ . This volume fraction should be used for any calculation of the interparticle structure factor (and is already done for you in models that combine this vesicle model with  $S(q)$  models).

The macro provided, `Vesicle_Volume_N_Rg()`, calculates the volume of the vesicle, the number density of vesicles, the excluded volume of the vesicles, along with  $I(q=0)$  and  $R_g$ .

For a general core-shell sphere,  $R_g$  is given by:

$$R_g^2 = \frac{3}{5} R_2^2 \left\{ \frac{\left( \frac{(\rho_1 - \rho_2)}{(\rho_2 - \rho_{\text{solv}})} \frac{R_1^5}{R_2^5} - 1 \right)}{\left( \frac{(\rho_1 - \rho_2)}{(\rho_2 - \rho_{\text{solv}})} \frac{R_1^3}{R_2^3} - 1 \right)} \right\}$$

$R_1$  and  $R_2$  are as defined above, and denote the core radius and the total radius, respectively. So for vesicle with  $\text{SLD}(1) = \text{SLD}(\text{solvent})$ , this reduces to:

$$R_g^2 = \frac{3}{5} R_2^2 \left\{ \frac{\left( \frac{R_1^5}{R_2^5} + 1 \right)}{\left( \frac{R_1^3}{R_2^3} + 1 \right)} \right\}$$

The scattered intensity at  $q=0$  is given by:

$$I(q=0) = n V_{shell}^2 (\rho_{shell} - \rho_{solv})^2$$

Note that  $I(q=0)$  for a vesicle depends only on the volume of the shell, not the overall volume of the vesicle.  $I(0)$  depends on the "dry" volume of scattering particles and does not depend on solvation, or how much the particle is swollen with solvent. This applies to any particle swollen with solvent.

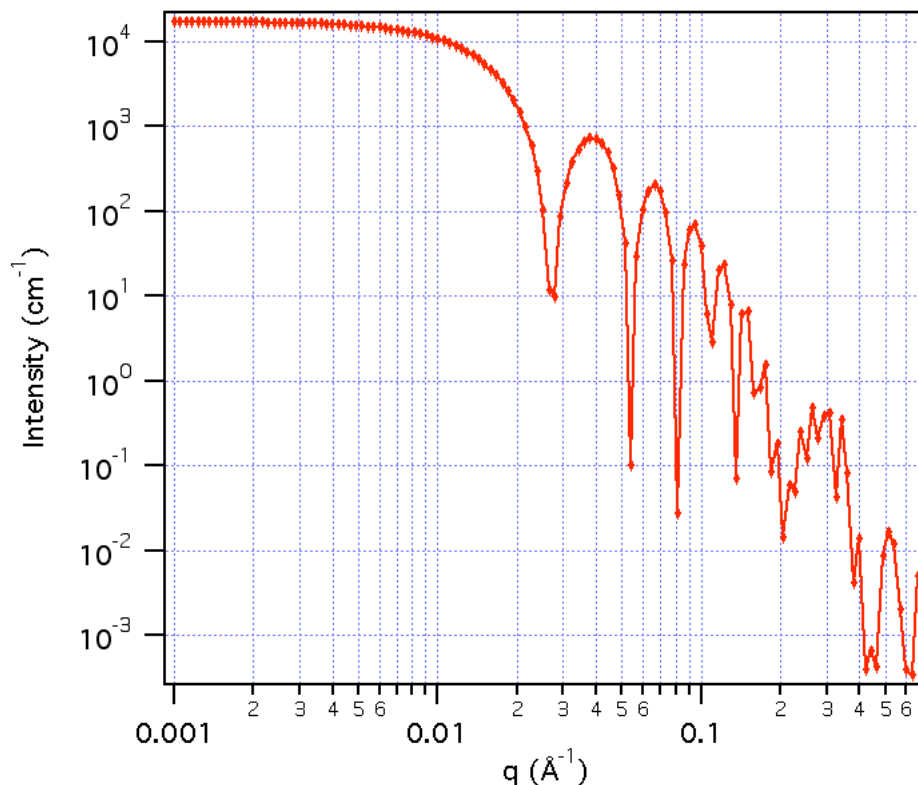
$w[0]$  (scale) and the contrast ( $=$  solvent SLD - shell SLD) are multiplicative factors in the model and are perfectly correlated. No more than one of these parameters can be free during the model fitting.

## REFERENCE

Guinier, A. and G. Fournet, "Small-Angle Scattering of X-Rays", John Wiley and Sons, New York, (1955).

## TEST DATASET

This example dataset is produced by running the Macro PlotVesicle(), using 128 data points,  $q_{min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_vesicle values.



## Multilamellar Vesicles

MACRO : FUNCTION

PlotMultiShellSphere() : MultiShellForm(w,y,x)

Wave extension: \_mss

File:

MultiShell.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

#### **AUTHOR/MODIFICATION**

Steve Kline 06 NOV 1998

#### **APPROVED FOR DISTRIBUTION**

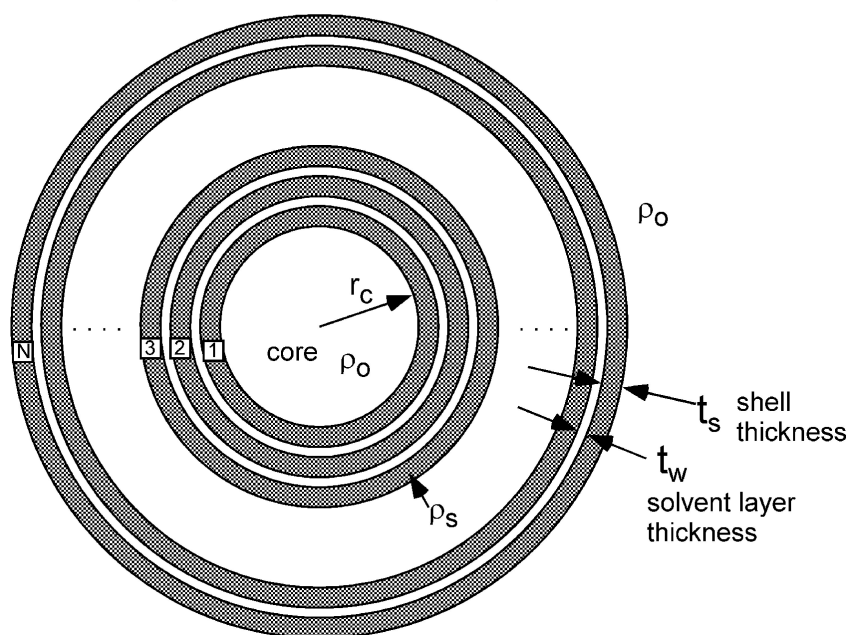
Charlie Glinka 21 NOV 2003

#### **DESCRIPTION**

Calculates the form factor for monodisperse spherical particles made up of a solvent-filled core with N shells. The shells are interleaved with layers of solvent. For N=1, this is a model for a unilamellar vesicle, i.e. solvent core plus one shell (representing, e.g. a lipid bilayer), and surrounded by solvent. N > 1 corresponds to a multilamellar vesicle.

### **Multi-Shell Spherical Model**

(e.g. multilamellar vesicles)



The resolution smeared version gives the most appropriate view of the model. Note that the resolution smearing calculation uses 76 Gauss quadrature points to properly smear the model since the function is HIGHLY oscillatory, especially around the q-values that correspond to the repeat distance of the layers. This can make the calculations rather slow.

#### **VARIABLES**

Input Variables (default values):

Point	parameters_mss	coef_mss
0	scale	1
1	core radius (A)	60
2	shell thickness (A)	10
3	water thickness	10
4	core & solvent SLD (A-2)	6.4e-06
5	Shell SLD (A-2)	4e-07
6	number of water/shell pairs	2
7	bkg (cm-1)	0.001

## USAGE NOTES

The value returned by the fitting routine for the number of water/shell pairs will be a floating point number. The physical reality must be an integer number of layers. In the model function, the value is truncated so that only the integer portion is used. That is 5.95 "pairs" is actually calculating the scattering for 5 pairs.

The returned value is scaled to units of  $[\text{cm}^{-1}]$

If the scale factor  $w[0]$  is set equal to the particle volume fraction,  $\phi$ , then the returned value is the scattered intensity per unit volume,  $I(q) = \phi * P(q)$ . However, no interparticle interference effects are included in this calculation.

### IMPORTANT:

This is a highly non-linear model function, complicated by the fact that the number of water/shell pairs must physically be an integer value, although the optimization treats it as a floating point value. For the best possible experience:

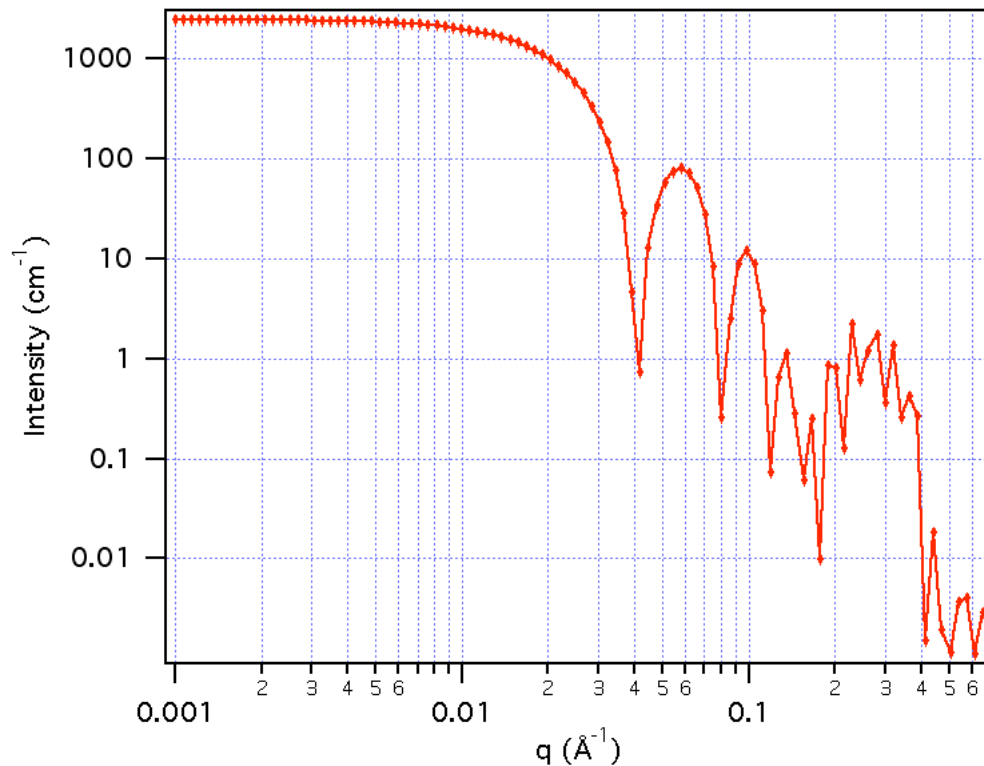
- Start with the best possible guess
- Using a priori knowledge, hold as many parameters fixed as possible
- if  $N=1$ ,  $tw$  (water thickness) must by definition be zero. Both  $N$  and  $tw$  must be fixed during fitting.
- If  $N > 1$ , use constraints to keep  $N > 1$  (set this up in the curve fitting dialog)
- To force  $N$  to "move" during fitting, you may need to set an "epsilon" wave to force a larger step in that direction.  $\epsilon = 0.001$  is good for all parameters other than  $N$ , which should be set to 1. (set this up in the curve fitting dialog)

## REFERENCE

Cabane, B., Small Angle Scattering Methods, *Surfactant Solutions: New Methods of Investigation*, Ch.2, Surfactant Science Series Vol. 22, Ed. R. Zana, M. Dekker, New York, 1987.

## TEST DATASET

This example dataset is produced by running the Macro PlotMultiShellSphere(), using 100 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_mss values.

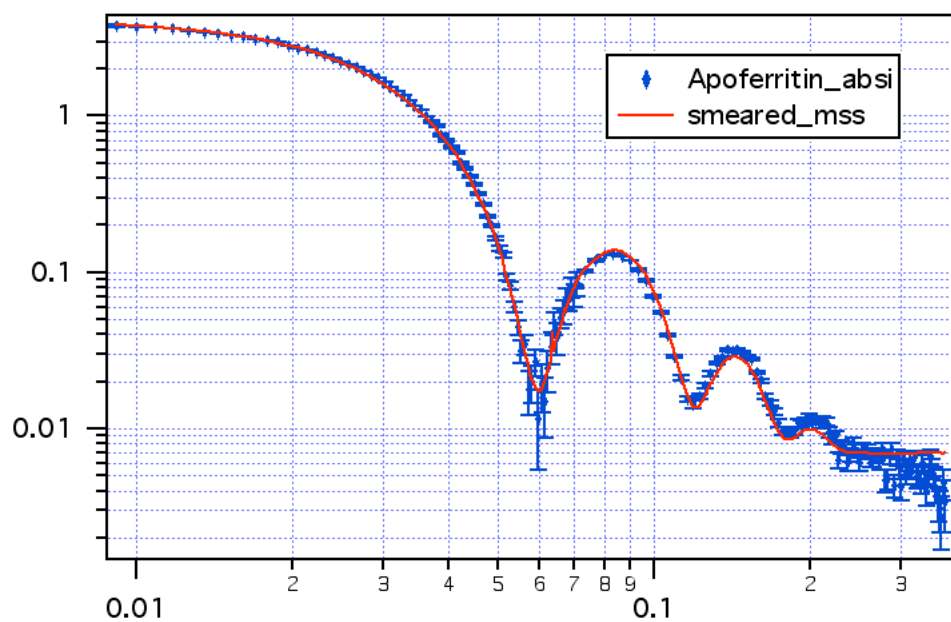


As a further example, shown below is a fit of SANS data for a 1.0 vol % solution of the nearly spherical, hollow protein Apoferritin in D<sub>2</sub>O, using the multi-spherical shell model. These same data are used in the SANS Data Analysis Tutorial, where a Spherical Core-Shell Model is shown to fit the data quite well.

Here the smeared multi-spherical shell is used to obtain an equally good fit. In fact, the two are numerically identical. In the fitting, the fixed parameters are: N (number of shells) = 1;  $t_w$  (water layer thickness) = 0; core and solvent SLD (D<sub>2</sub>O) =  $6.4 \times 10^{-6} \text{ Å}^{-2}$ ; and, particle volume fraction (scale) = 0.01.

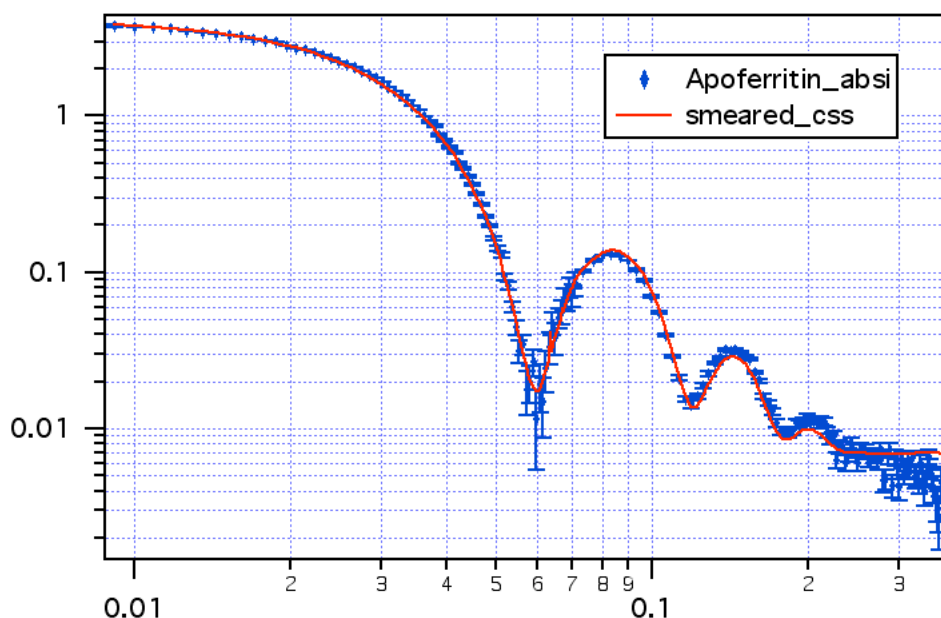
Shown below are the fits and the fitted parameters for each model.

**Multi-Spherical Shell model fit to SANS Apoferritin data.**



Point	smear_parameters_mss	smear_coef_mss	W_sigma
0	scale	0.01	0
1	core radius (A)	40.6876	0.0643463
2	shell thickness (A)	22.8046	0.100453
3	water thickness (A)	0	0
4	core & solvent SLD (A-2)	6.4e-06	0
5	Shell SLD (A-2)	3.71054e-06	8.09284e-09
6	number of water/shell pairs	1	0
7	bkg (cm-1)	0.00678103	9.07204e-05

**Spherical Core-Shell model fit to SANS Apoferritin data** (see SANS Data Analysis Tutorial for details).



Point	smear_parameters_css	smear_coef_css	W_sigma
0	scale	0.01	0
1	core radius (A)	40.686	0.0643462
2	shell thickness (A)	22.807	0.100449
3	Core SLD (A-2)	6.4e-06	0
4	Shell SLD (A-2)	3.71073e-06	8.09075e-09
5	Solvent SLD (A-2)	6.4e-06	0
6	bkg (cm-1)	0.00678223	9.0715e-05

### Polydisperse Core with Constant Shell Thickness

#### **MACRO : FUNCTION**

PlotPolyCoreForm() : PolyCoreForm(w,y,x)

Wave extension: \_pcf

File:

PolyCore.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

#### **AUTHOR/MODIFICATION**

Steve Kline 06 NOV 1998

#### **APPROVED FOR DISTRIBUTION**

Sungmin Choi 02 FEB 1999

#### **DESCRIPTION**

Calculates the form factor for polydispersed spherical particles with a core-shell structure. The spherical particles have a polydisperse core with a constant shell thickness. The form factor is normalized by the average particle volume such that

$P(q) = \text{scale} \cdot \langle f^2 \rangle / \text{Vol} + \text{bkg}$ , where  $f$  is the single particle scattering amplitude, appropriately averaged over the Schulz distribution of radii. Resolution smeared version is also provided.

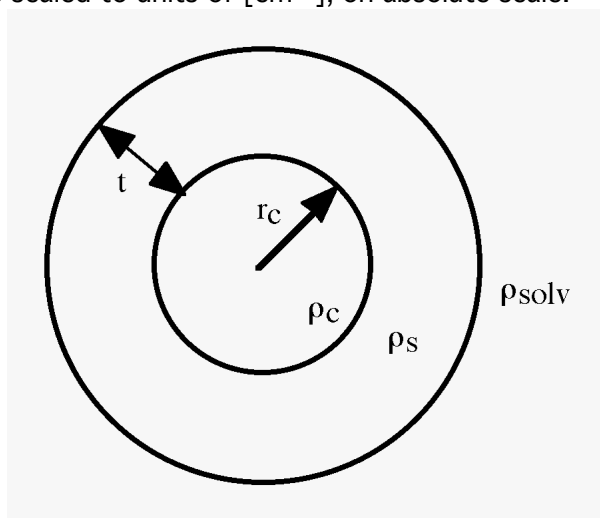
## VARIABLES

Input Variables (default values):

Point	parameters_pcf	coef_pcf
0	scale	1
1	avg core rad (A)	60
2	core polydisp (0,1)	0.2
3	shell thickness (A)	10
4	SLD core (A-2)	1e-06
5	SLD shell (A-2)	2e-06
6	SLD solvent (A-2)	3e-06
7	bkg (cm-1)	0.001

## USAGE NOTES

The returned value is scaled to units of  $[\text{cm}^{-1}]$ , on absolute scale.



$w[0]$  (scale) is correlated with the SLD's that describe the particle. No more than one of these parameters can be free during model fitting.

$w[2]$  (polydispersity) may need to be constrained to keep it within its physical limits of (0,1). Polydispersity,  $p = \sigma/R_c$ , where  $\sigma^2$  is the variance of the distribution and  $R_c$  is the mean core radius,  $\text{coef\_pcf}[1]$ . For a more complete description of the Schulz distribution, see: J. Hayter in "Physics of Amphiphiles - Micelles, Vesicles and Microemulsions" V. DeGiorgio and M. Corti, Eds. (1983) p. 69.

The returned form factor is normalized by the average particle volume  $\langle V \rangle$ :

$$\langle V \rangle = \frac{4\pi}{3} \langle r^3 \rangle \quad \text{where} \quad \langle r^3 \rangle = \frac{(z+3)(z+2)}{(z+1)^2} \langle r \rangle$$



and  $z$  is the width parameter of the Schulz distribution,  $z = (1/p^2) - 1$ .

Setting the SLD of the core and shell equal to simulate a uniform sphere results in a mathematical (divide by zero) error - and no model is plotted. To simulate a uniform SLD sphere, set the shell thickness to zero (the SLD of the shell will now make no contribution to the scattering).

The average particle diameter is  $2 \times (\text{Radius} + \text{shell thickness})$

If the scale factor  $w[0]$  is set equal to the particle volume fraction,  $\phi$ , the returned value is the scattered intensity per unit volume,  $I(q) = \phi \cdot P(q)$ .

No interparticle interference effects are included in this calculation.

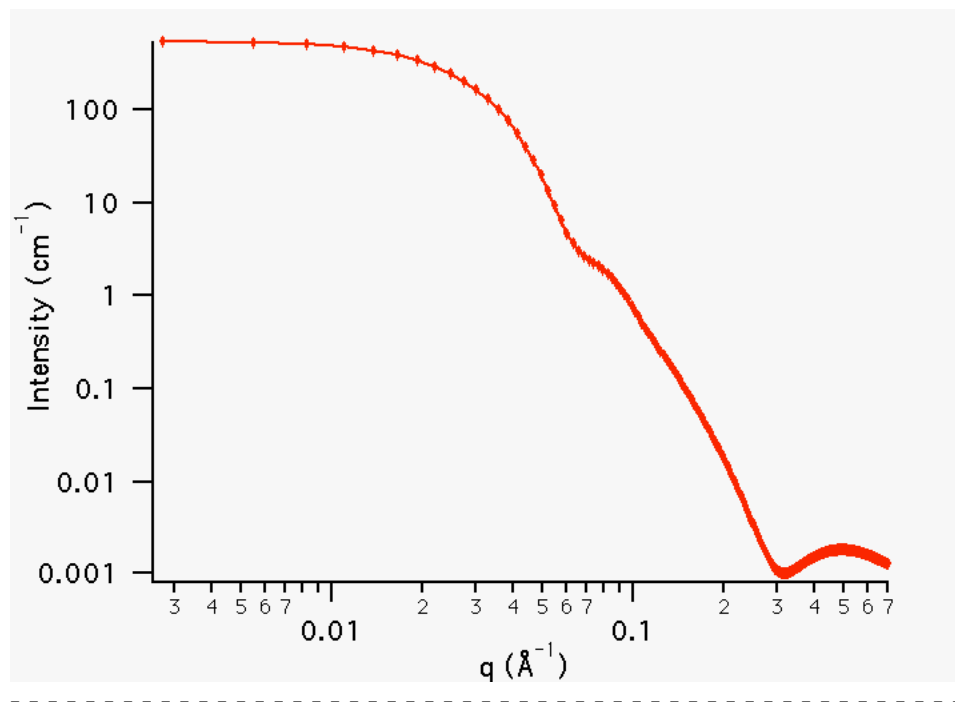
This function is useful for vesicles or liposomes by setting the SLD (core) = SLD (solvent), thus calculating scattering from a spherical shell with constant thickness, but polydisperse inner radius.

## REFERENCE

Bartlett, P.; Ottewill, R. H. *J. Chem. Phys.*, **1992**, *96*, 3306.

## TEST DATASET

This example dataset is produced by running the Macro PlotPolyCoreForm(), using 256 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_pcf values.



## Core-Shell with Constant Core/Shell Ratio

**MACRO : FUNCTION**

PlotPolyCoreShellRatio() : PolyCoreShellRatio(w,y,x)

Wave extension:       \_pcr

File:

PolyCoreShellRatio.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

**AUTHOR/MODIFICATION**

Steve Kline    06 NOV 1998

**APPROVED FOR DISTRIBUTION**

Sungmin Choi 02 FEB 1999

**DESCRIPTION**

Calculates the form factor for a polydisperse spherical particle with a core-shell structure. In this model, the ratio  $R(\text{core})/R(\text{core+shell})$  is held constant. The form factor is normalized by the mean particle volume such that  $P(q) = \text{scale} \cdot \langle f^2 \rangle / \text{Vol} + \text{bkg}$ , where  $f$  is the single particle scattering amplitude and the average  $\langle \rangle$  is over a Schulz distribution of radii. Resolution smeared version is also provided.

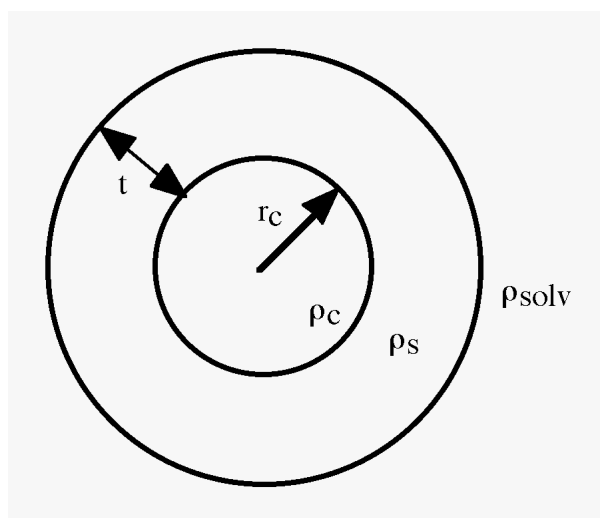
**VARIABLES**

Input Variables (default values):

Point	parameters_pcr	coef_pcr
0	scale	1
1	avg core rad (Å)	60
2	avg shell thickness (Å)	10
3	overall polydisp (0,1)	0.2
4	SLD core (Å <sup>-2</sup> )	1e-06
5	SLD shell (Å <sup>-2</sup> )	2e-06
6	SLD solvent (Å <sup>-2</sup> )	3e-06
7	bkg (cm <sup>-1</sup> )	0.001

**USAGE NOTES**

The returned value is scaled to units of [cm<sup>-1</sup>], on absolute scale.



w[0] (scale) is correlated with the SLD's that describe the particle. No more than one of these parameters can be free during model fitting.

w[2] (polydispersity) may need to be constrained to keep it within its physical limits of (0,1). Polydispersity,  $p = \sigma/Rt$ , where  $\sigma^2$  is the variance of the distribution and  $Rt$  is the total particle radius,  $Rt = R_c + t$ . For a more complete description of the Schulz distribution, see: J. Hayter in "Physics of Amphiphiles - Micelles, Vesicles and Microemulsions" V. DeGiorgio and M. Corti, Eds. (1983) p. 69.

The returned form factor is normalized by the average particle volume  $\langle V \rangle$ :

$$\langle V \rangle = \frac{4\pi}{3} \langle r^3 \rangle \quad \text{where} \quad \langle r^3 \rangle = \frac{(z+3)(z+2)}{(z+1)^2} \langle r \rangle \quad \text{and here } r \text{ denotes the total particle radius, } R_c + t, \text{ and } z \text{ is the width parameter of the Schulz distribution, } z = (1/p^2) - 1.$$

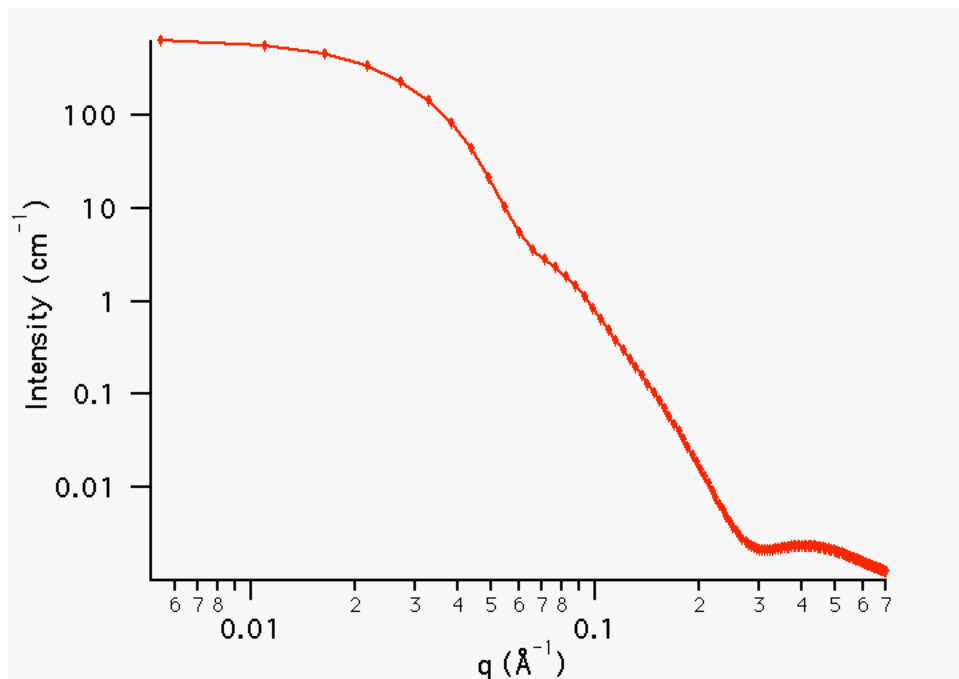
If the scale factor w[0] is set equal to the particle volume fraction,  $\phi$ , the returned value is the scattered intensity per unit volume,  $I(q) = \phi * P(q)$ . However, no interparticle interference effects are included in this calculation.

## REFERENCE

J. B. Hayter in "Physics of Amphiphiles--Micelles, Vesicles, and Microemulsions" Eds. V. DeGiorgio; M. Corti, pp. 59-93, 1983. Eqns: 32-37

## TEST DATASET

This example dataset is produced by running the Macro PlotPolyCoreShellRatio(), using 128 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_pcr values.



### Spheres with Rectangular Size Distribution

#### **MACRO : FUNCTION**

PlotPolyRectSpheres() : PolyRectSpheres(w,y,x)

Wave extension: \_rect

File:

PolyRectSphere.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

#### **AUTHOR/MODIFICATION**

Steve Kline 20 JAN 1999

#### **APPROVED FOR DISTRIBUTION**

Sungmin Choi 02 FEB 1999

#### **DESCRIPTION**

Calculates the form factor for a polydisperse population of spheres with uniform scattering length density. The distribution of radii is a rectangular (box) distribution. The form factor is normalized by the average particle volume such that  $P(q) = \text{scale} \cdot \langle F^2 \rangle / \text{Vol} + \text{bkg}$ , where  $F$  is the scattering amplitude of a sphere and the  $\langle \rangle$  denote an average over the size distribution. Resolution smeared version is also provided.

#### **VARIABLES**

Input Variables (default values):

parameters_rect	coef_rect
scale	1
Radius (A)	60
polydispersity	0.12
SLD sphere (A <sup>-2</sup> )	1e-06
SLD solvent (A <sup>-2</sup> )	6.3e-06
background (cm <sup>-1</sup> )	0

## USAGE NOTES

The returned value is scaled to units of [cm<sup>-1</sup>], absolute scale.

contrast = SLD (sphere) - SLD (solvent)

The (normalized) rectangular distribution is:

$$f(r) = \begin{cases} \frac{1}{2w} & |r - R| \leq w \\ 0 & |r - R| > w \end{cases}$$

with the constraint that  $w \leq R$ . Here  $R$  is the average radius specified by coef[1] above.

$R$  is the mean of the distribution and  $w$  is the half-width. The root mean square deviation is  $\sigma_R = w/\sqrt{3}$ . The polydispersity,  $p = \sigma_R/R$ .

The form factor is normalized by the average volume, using

$$\langle V \rangle = \frac{4\pi}{3} \langle R^3 \rangle = \frac{4\pi}{3} \langle R \rangle^3 (1 + 3p^2)$$

The intensity at  $q=0$  is given by:

$$I(q=0) = \phi \Delta\rho^2 \frac{4\pi}{3} R^3 (1 + 3p^2)$$

and the (polydisperse) radius of gyration is:

$$R_g^2 = \frac{3}{5} \frac{\langle R^8 \rangle}{\langle R^6 \rangle} = \frac{3}{5} R^2 \frac{(1 + 28p^2 + 126p^4 + 108p^6 + 27p^8)}{(1 + 15p^2 + 27p^4 + (27/7)p^6)}$$

If the scale factor w[0] is set equal to the particle volume fraction,  $\phi$ , the returned value is the scattered intensity per unit volume,  $I(q) = \phi^*P(q)$ . However, no interparticle interference effects are included in this calculation.

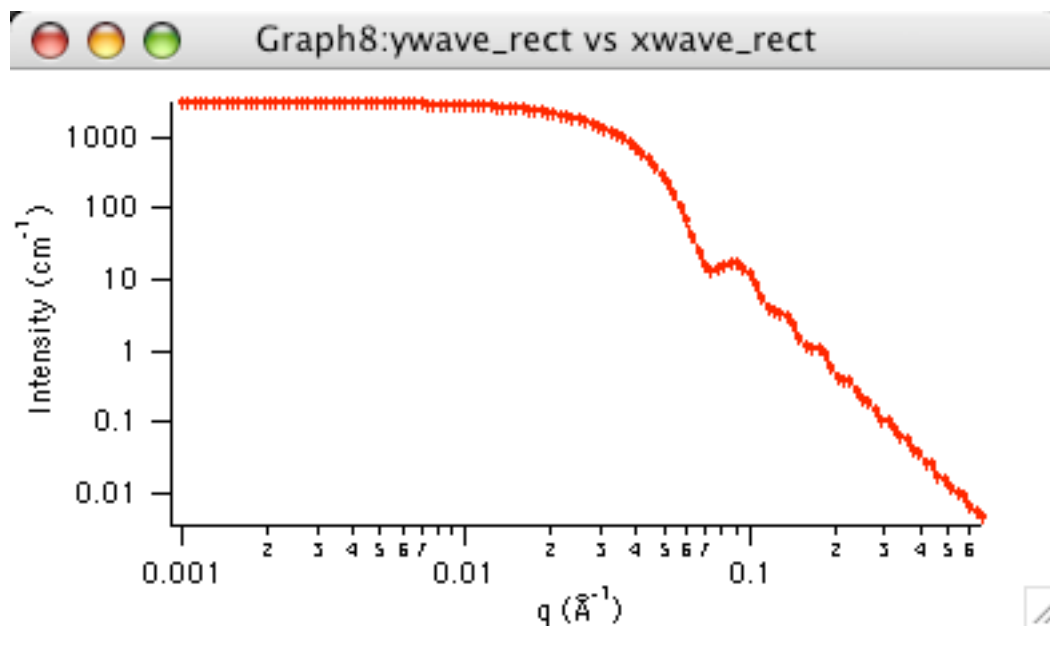
w[0] (scale) and contrast are multiplicative factors in the model and are perfectly correlated. Only one of these parameters should be left free during model fitting.

## REFERENCE

Kotlarchyk, M.; Chen, S.-H. *J. Chem. Phys.*, **1983**, 79, 2461.

## TEST DATASET

This example dataset is produced by running the Macro PlotPolyRectSpheres(), using 128 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_rect values.



## Spheres with Gaussian Size Distribution

### MACRO : FUNCTION

PlotGaussPolySphere() : GaussPolySphere(w,y,x)

NumberDensity\_Gauss()

PlotGaussDistribution()

Wave extension:     \_pgs

File:

GaussSpheres.ipf

Requires:

GaussUtils.ipf

[Sphere.ipf](#)

### AUTHOR/MODIFICATION

Steve Kline   12 SEP 2002

### APPROVED FOR DISTRIBUTION

John Barker   15 DEC 2003

### DESCRIPTION

Calculates the scattering for a polydisperse population of spheres with uniform scattering length density. The distribution of radii is a Gaussian (normal) distribution. The intensity is normalized by the average particle volume such that  $I(q) = \text{scale} \cdot \langle F^2 \rangle / \langle \text{Vol} \rangle + \text{bkg}$ , where  $F$  is the scattering amplitude of a sphere and the  $\langle \rangle$  denote an average over the size distribution. Resolution smeared version is also

provided.

Additionally, two macros are provided to (1) calculate the number density based on the volume fraction and polydisperse particle volume (weighted using the 3rd moment of the radius) and (2) plot the normalized probability distribution as a function of radius.

## VARIABLES

Input Variables (default values):

parameters_pgs	coef_pgs
Volume Fraction (scale)	0.01
mean radius (Å)	60
polydisp (sig/avg)	0.2
SLD sphere (Å <sup>-2</sup> )	1e-06
SLD solvent (Å <sup>-2</sup> )	3e-06
bkg (cm <sup>-1</sup> sr <sup>-1</sup> )	0.001

## USAGE NOTES

The returned value is scaled to units of [cm<sup>-1</sup> sr<sup>-1</sup>], absolute scale.

The (normalized) Gaussian distribution is:

$$f(R) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2\sigma^2}(R - R_{\text{avg}})^2\right]$$

Here  $R_{\text{avg}}$  is the average radius specified by coef[1] above and the polydispersity,  $p = \sigma/R_{\text{avg}}$ . Note that the distribution can extend to negative radii for large polydispersity. In this case the calculated intensity will not be a true reflection of the size distribution. The distribution can be plotted for the radius and polydispersity in the coef\_pgs wave using the macro "PlotGaussDistribution()".

The  $N^{\text{th}}$  moment of size distribution is equal to

$$\langle R^N \rangle = R_{\text{avg}}^N (1 + A_2 P^2 + 3 \cdot A_4 P^4 + 3 \cdot 5 \cdot A_6 P^6 \dots)$$

where the coefficients  $A_i$  can be extracted from

$$(u + r)^N \equiv A_0 r^N + A_1 r^{N-1} u + A_2 r^{N-2} u^2 \dots$$

The form factor is normalized by the average volume, using

$$\langle V \rangle = \frac{4\pi}{3} \langle R^3 \rangle = \frac{4\pi}{3} \langle R \rangle^3 (1 + 3p^2)$$

If the scale factor w[0] is set equal to the particle volume fraction,  $\phi$ , the returned value is the differential macroscopic scattering cross-section (scattered cross-section per unit sample volume per unit solid angle).

$$I(q) = \left(\frac{4\pi}{3}\right)^2 N_0 \Delta\rho^2 \int_0^\infty f(R) R^6 F^2(qR) dR$$

where  $N_0$  is the total number of particles per unit volume, and  $\Delta\rho = w[3]-w[4]$ , is the difference in scattering length density. The number of particles per unit volume having size between  $R$  and  $R+dR$  is equal to  $N(R)dR = N_0 f(R)dR$ . The Macro PlotGaussDistribution plots the function  $f(R)$  vs  $R$ .

The scattering amplitude for a sphere is

$$F(x) = \frac{[\sin(x) - x \cos(x)]}{x^3}$$

However, no interparticle interference effects are included in this calculation. Interparticle interference  $S(q)$  should be included by

$$I(q) = N_0 S(q) P(q)$$

where  $P(q)$  is the form factor. Some other relations of interest are:

$$N_0 = \phi / \langle V \rangle$$

Guinier radius:

$$R_G = \sqrt{\frac{3\langle R^8 \rangle}{5\langle R^6 \rangle}} = R_{avg} \sqrt{\frac{3}{5}} \frac{(1 + 28p^2 + 210p^4 + 420p^6 + 105p^8)}{(1 + 15p^2 + 45p^4 + 15p^6)}$$

Total interfacial surface area per unit sample volume:

$$S_V = 4\pi \langle R^2 \rangle N_0 = 3\phi \frac{\langle R^2 \rangle}{\langle R^3 \rangle} = \frac{3\phi}{R_{avg}} \frac{(1 + p^2)}{(1 + 3p^2)}$$

The forward scattering cross-section:

$$I(0) = N_0 \langle V^2 \rangle \Delta\rho^2 = \frac{4}{3} \pi \phi \Delta\rho^2 \frac{\langle R^6 \rangle}{\langle R^3 \rangle} = \frac{4}{3} \pi \phi \Delta\rho^2 R_{avg}^3 \frac{(1 + 15p^2 + 45p^4 + 15p^6)}{(1 + 3p^2)}$$

These values are calculated using the macro "NumberDensity\_Gauss()" and use the current values in the coef\_pgs wave.

$W[0]$  (volume fraction or arbitrary scale) and  $(W[3]-W[4])^2$  (contrast) are multiplicative factors in the model and are perfectly correlated. Only one of these three parameters should be left free during model fitting.

## REFERENCE

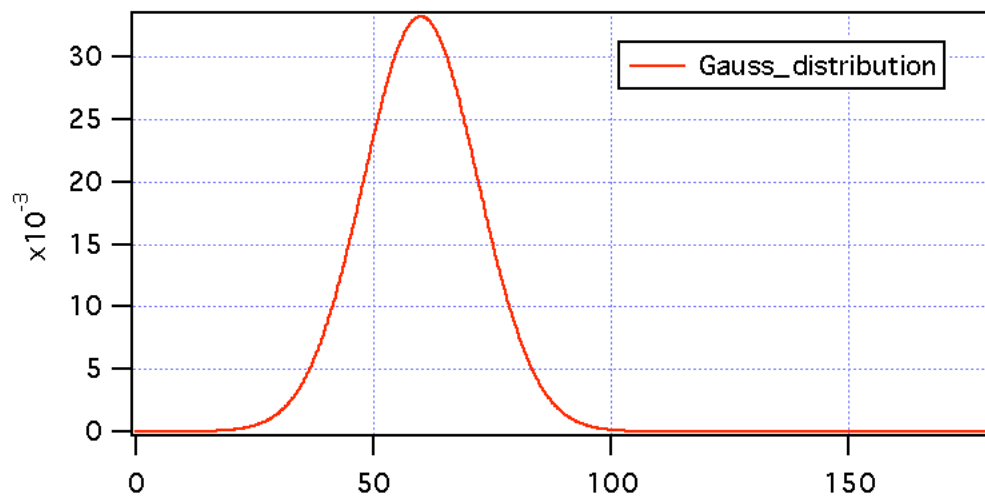
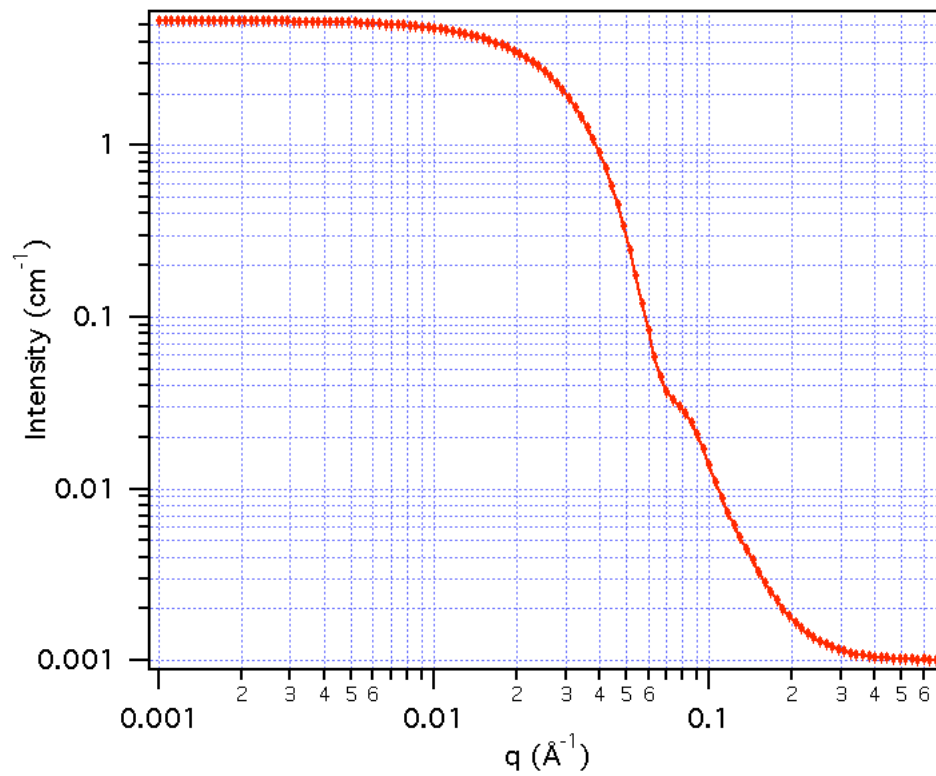
none.

## TEST DATASET

This example dataset is produced by running the Macro PlotGaussPolySphere(), using 128 data points,  $q_{min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_pgs



values.



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### Spheres with Log-Normal Size Distribution

**MACRO : FUNCTION**

PlotLogNormalPolySphere() : LogNormalPolySphere(w,y,x)

NumberDensity\_LogN()

PlotLogNormalDistribution()

Wave extension:      \_Ins

File:

LogNormalSphere.ipf

Requires:

GaussUtils.ipf

[Sphere.ipf](#)

## AUTHOR/MODIFICATION

Steve Kline    12 SEP 2002

## APPROVED FOR DISTRIBUTION

John Barker    10 Nov 2003

## DESCRIPTION

Calculates the scattering for a polydisperse population of spheres with uniform scattering length density. The distribution of radii is a LogNormal distribution. The intensity is normalized by the average particle volume such that  $I(q) = \text{scale} \cdot \langle F^2 \rangle / \langle \text{Vol} \rangle + \text{bkg}$ , where  $F$  is the scattering amplitude of a sphere and the  $\langle \rangle$  denote an average over the size distribution. Resolution smeared version is also provided.

Additionally, two macros are provided to (1) calculate the number density based on the volume fraction and polydisperse particle volume (weighted using the 3rd moment of the radius) and (2) plot the normalized probability distribution as a function of radius.

## VARIABLES

Input Variables (default values):

Point	parameters_Ins	coef_Ins
0	Volume Fraction (scale)	0.01
1	$\exp(\mu) = \text{median Radius (A)}$	60
2	$\sigma$	0.2
3	SLD sphere (A <sup>-2</sup> )	1e-06
4	SLD solvent (A <sup>-2</sup> )	2e-06
5	bkg (cm <sup>-1</sup> sr <sup>-1</sup> )	0

## USAGE NOTES

The returned value is scaled to units of  $[\text{cm}^{-1} \text{s r}^{-1}]$ , absolute scale.

The (normalized) LogNormal distribution is:

$$f(R) = \frac{1}{\sigma R \sqrt{2\pi}} \exp \left[ -\frac{1}{2\sigma^2} (\ln(R) - \mu)^2 \right]$$

Here  $\mu = \ln(R_{\text{med}})$ , where  $R_{\text{med}}$  is the median radius specified by W[1] above and the polydispersity is given by  $\sigma$ . Note that the distribution is strictly positive for any

polydispersity. The distribution can be plotted for the radius and polydispersity in the coef\_lns wave using the macro "PlotLogNormalDistribution()".

The  $N^{\text{th}}$  moment of size distribution is equal to

$$\langle R^N \rangle = \exp(N\mu + N^2\sigma^2 / 2)$$

The form factor is normalized by the average volume, using the 3rd moment of R:

$$\langle V \rangle = \frac{4\pi}{3} \langle R^3 \rangle = \frac{4\pi}{3} \exp\left(3\mu + \frac{9}{2}\sigma^2\right)$$

If the scale factor  $W[0]$  is set equal to the particle volume fraction,  $\phi$ , the returned value is the differential macroscopic scattering cross-section (scattered cross-section per unit sample volume per unit solid angle).

$$I(q) = \left(\frac{4\pi}{3}\right)^2 N_0 \Delta\rho^2 \int_0^\infty f(R) R^6 F^2(qR) dR$$

where  $N_0$  is the total number of particles per unit volume, and  $\Delta\rho = w[3]-w[4]$ , is the difference in scattering length density. The number of particles per unit volume having size between  $R$  and  $R+dR$  is equal to  $N(R)dR = N_0 f(R)dR$ . The Macro PlotLogNormalDistribution plots the function  $f(R)$  vs  $R$ .

The scattering amplitude for a sphere is

$$F(x) = \frac{[\sin(x) - x \cos(x)]}{x^3}$$

However, no interparticle interference effects are included in this calculation. Interparticle interference  $S(q)$  should be included by

$$I(q) = N_0 S(q) P(q)$$

where  $P(q)$  is the form factor. Some other relations of interest are:

$$N_0 = \phi / \langle V \rangle$$

The mean radius:

$$R_{avg} = \exp(\mu + \sigma^2 / 2)$$

The peak in the size distribution occurs at radius:

$$R_{pk} = \exp(\mu - \sigma^2)$$

Guinier radius:

$$R_G = \sqrt{\frac{3\langle R^2 \rangle}{5\langle R^2 \rangle}} = \exp(2\mu + 14\sigma^2) \sqrt{\frac{3}{5}}$$

Total interfacial surface area per unit sample volume:

$$S_V = 4\pi\langle R^2 \rangle N_0 = 3\phi \exp\left(-\mu - \frac{5}{2}\sigma^2\right)$$

The forward scattering cross-section:

$$I(0) = N_0\langle V^2 \rangle \Delta\rho^2 = \frac{4}{3}\pi\phi\Delta\rho^2 \exp\left(3\mu + \frac{27}{2}\sigma^2\right)$$

These values are calculated using the macro "NumberDensity\_LogN()" and use the current values in the coef\_Ins wave.

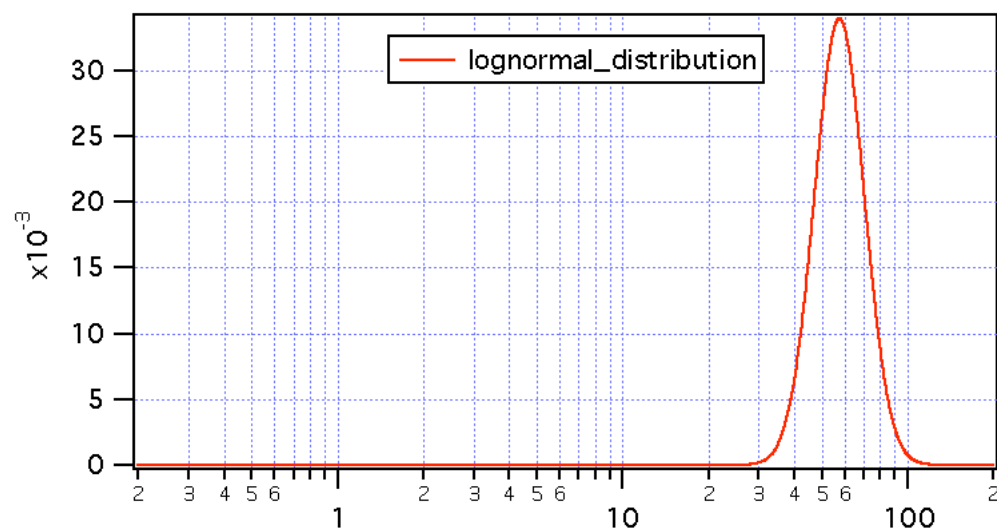
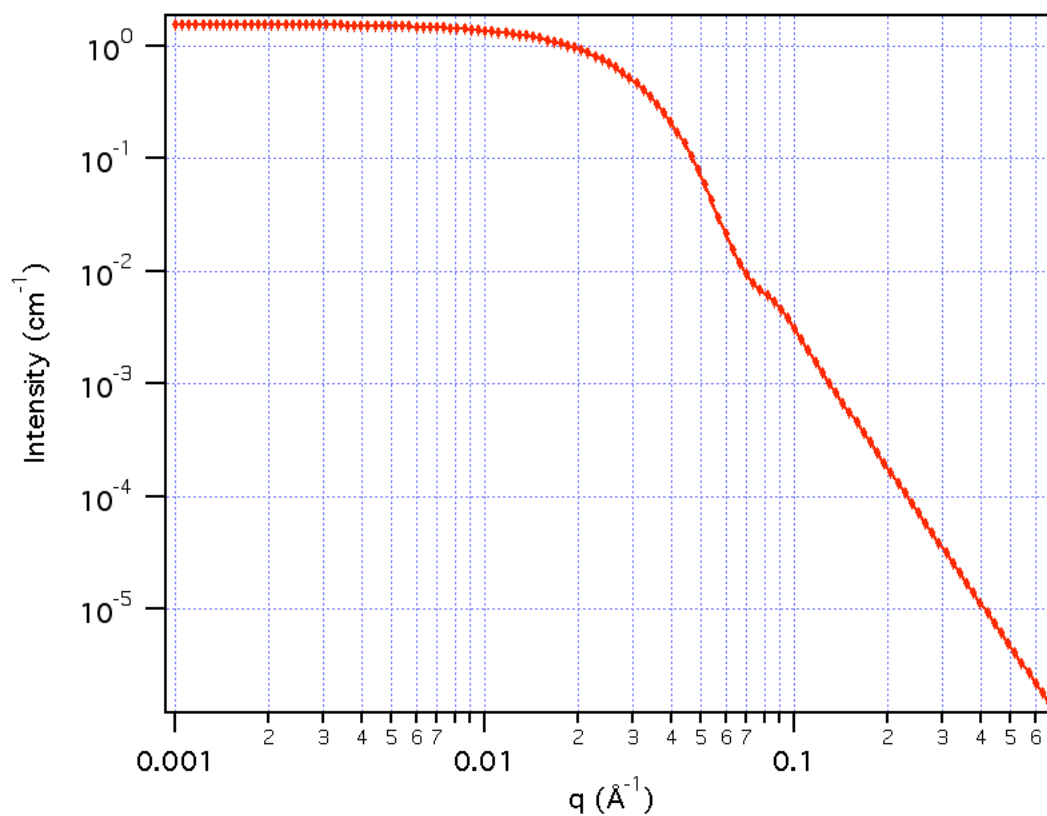
W[0] (volume fraction or arbitrary scale) and  $(W[3]-W[4])^2$  (contrast) are multiplicative factors in the model and are perfectly correlated. Only one of these three parameters should be left free during model fitting.

## REFERENCE

none.

## TEST DATASET

This example dataset is produced by running the Macro PlotLogNormalPolySphere(), using 128 data points,  $q_{min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_Ins values.



### Spheres with Schulz Size Distribution

**MACRO : FUNCTION**

PlotSchulzPolySpheres() : SchulzSpheres(w,y,x)

NumberDensity\_Schulz()

PlotSchulzDistribution()

Wave extension :     \_sch

File: SchulzSpheres.ipf  
 Requires: GaussUtils.ipf

**AUTHOR/MODIFICATION**  
 Steve Kline 12 SEP 2002

**APPROVED FOR DISTRIBUTION**  
 John Barker 6 Nov 2003

## DESCRIPTION

Calculates the scattering for a polydisperse population of spheres with uniform scattering length density. The distribution of radii is a Schulz distribution. The Intensity is normalized by the average particle volume such that  $I(q) = \text{scale} \cdot \langle F^2 \rangle / \langle \text{Vol} \rangle + \text{bkg}$ , where  $F$  is the scattering amplitude of a sphere and the  $\langle \rangle$  denote an average over the size distribution. Resolution smeared version is also provided.

Additionally, two macros are provided to (1) calculate the number density based on the volume fraction and polydisperse particle volume (weighted using the 3rd moment of the radius) and (2) plot the normalized probability distribution as a function of radius.

## VARIABLES

Input Variables (default values):

Point	parameters_sch	coef_sch
0	Volume Fraction (scale)	0.01
1	mean radius (A)	60
2	polydisp (sig/avg)	0.2
3	SLD sphere (A-2)	1e-06
4	SLD solvent (A-2)	3e-06
5	bkg (cm-1 sr-1)	0.001

## USAGE NOTES

The returned value is scaled to units of  $[\text{cm}^{-1} \text{sr}^{-1}]$ , absolute scale.

The (normalized) Schulz distribution is:

$$f(R) = (z+1)^{z+1} x^z \frac{\exp[-(z+1)x]}{R_{\text{avg}} \Gamma(z+1)}$$

where  $R_{\text{avg}}$  is the mean radius specified by  $W[1]$  above and  $x = R/R_{\text{avg}}$ ,  $z$  is related to the polydispersity,  $p = \sigma/R_{\text{avg}}$ , by  $z = 1/p^2 - 1$ .  $\sigma^2$  is the variance of the distribution. The distribution can be plotted for the radius and polydispersity in the coef\_sch wave using the macro "PlotSchulzDistribution()".

The  $N^{\text{th}}$  moment of size distribution is equal to

$$\langle R^N \rangle = \frac{R_{\text{avg}}^N}{(z+1)^N} \frac{(z+N)!}{z!}$$

The form factor is normalized by the average volume, using the 3<sup>rd</sup> moment of R:

$$\langle V \rangle = \frac{4\pi}{3} \langle R^3 \rangle = \frac{4\pi}{3} \langle R_{\text{avg}} \rangle^3 \frac{(z+3)(z+2)}{(z+1)^2}$$

If the scale factor  $W[0]$  is set equal to the particle volume fraction,  $\phi$ , the returned value is the differential macroscopic scattering cross-section (scattered cross-section per unit sample volume per unit solid angle).

$$I(q) = \left(\frac{4\pi}{3}\right)^2 N_0 \Delta\rho^2 \int_0^\infty f(R) R^6 F^2(qR) dR$$

where  $N_0$  is the total number of particles per unit volume, and  $\Delta\rho = w[3]-w[4]$ , is the difference in scattering length density. The number of particles per unit volume having size between  $R$  and  $R+dR$  is equal to  $N(R)dR = N_0 f(R)dR$ . The MacroPlotSchulzDistribution plots the function  $f(R)$  vs  $R$ .

The scattering amplitude for a sphere is

$$F(x) = \frac{[\sin(x) - x \cos(x)]}{x^3}$$

However, no interparticle interference effects are included in this calculation. Interparticle interference  $S(q)$  should be included by

$$I(q) = N_0 S(q) P(q)$$

where  $P(q)$  is the form factor. Some other relations of interest are:

$$N_0 = \phi / \langle V \rangle$$

Guinier radius:

$$R_g = \sqrt{\frac{3\langle R^8 \rangle}{5\langle R^6 \rangle}} = R_{\text{avg}} \sqrt{\frac{3(z+8)(z+7)}{5(z+1)^2}}$$

Total interfacial surface area per unit sample volume:

$$S_V = 4\pi \langle R^2 \rangle N_0 = \frac{3\phi}{R_{\text{avg}}} \frac{(z+1)}{(z+3)}$$

The forward scattering cross-section:

$$I(q=0) = N_o \langle V^2 \rangle \Delta\rho^2 = \phi \Delta\rho^2 \frac{4\pi}{3} R_{avg}^3 \frac{(z+6)(z+5)(z+4)}{(z+1)^3}$$

These values are calculated using the macro "NumberDensity\_Schulz()" and use the current values in the coef\_sch wave.

W[0] (volume fraction or arbitrary scale) and  $(W[3]-W[4])^2$  (contrast) are multiplicative factors in the model and are perfectly correlated. Only one of these three parameters should be left free during model fitting. W[2] (polydispersity (p)) must be between  $0 < p < 1$ .

NOTE that this calculation is an analytic solution and is much faster to compute than the Log Normal or Gaussian distributions of spheres which are both numerical solutions.

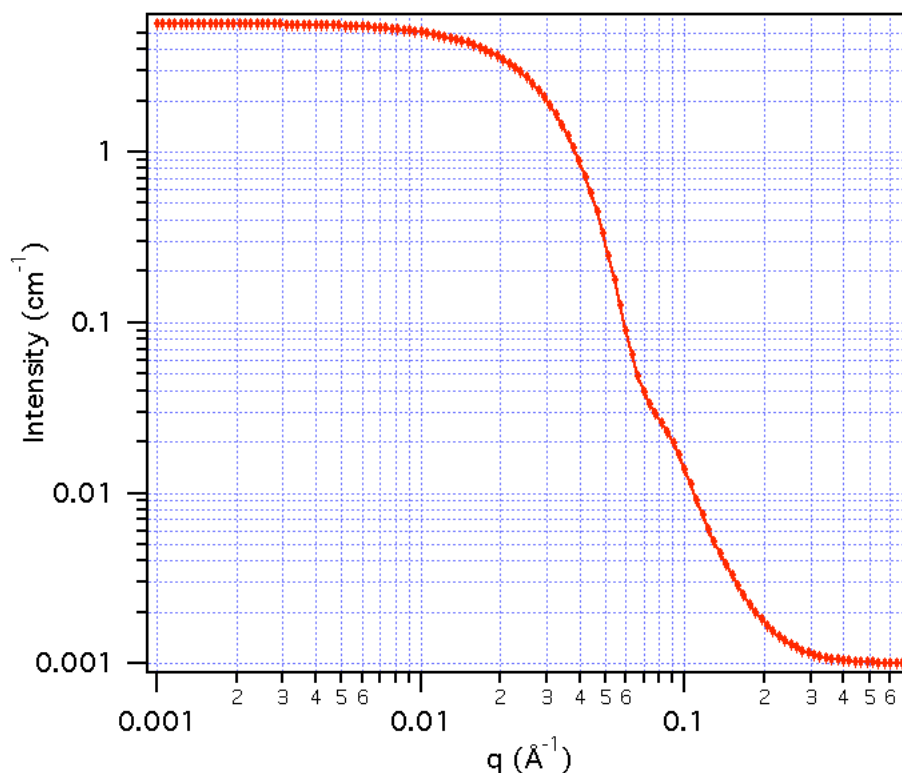
## REFERENCE

G. V. Schulz, *Z. Phys. Chem.*, **43** (1935) 25.

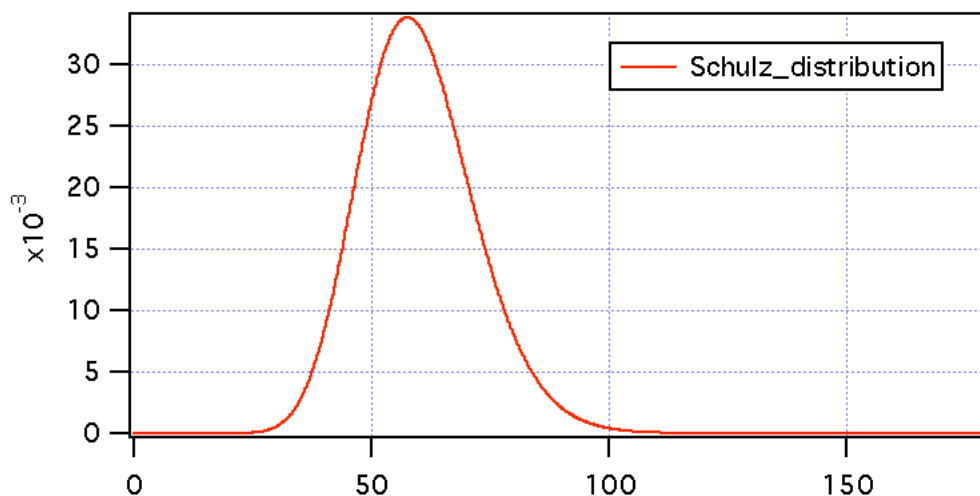
M. Kotlarchyk and S-H. Chen, *J. Chem. Phys.* **79** (1983) 2461-2469, eqn 25-29.

## TEST DATASET

This example dataset is produced by running the Macro PlotSchulzPolySpheres(), using 128 data points,  $q_{min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_sch values.







### Spheres with Bimodal Schulz Size Distribution

#### **MACRO : FUNCTION**

PlotBimodalSchulzSpheres() : BimodalSchulzSpheres(w,y,x)  
 NumberDensity\_Bimodal()  
 Plot\_Bimodal\_Distribution()

Wave extension :     \_bss

File:

BimodalSchulzSpheres.ipf

Requires:

SchulzSpheres.ipf

GaussUtils.ipf

#### **AUTHOR/MODIFICATION**

Steve Kline   12 SEP 2002

#### **APPROVED FOR DISTRIBUTION**

John Barker   6 NOV 2003

#### **DESCRIPTION**

Calculates the scattering for a bidisperse population of spheres with uniform scattering length density. Each population of spheres is polydisperse with a distribution of radii obeying a Schulz distribution. The Intensity is normalized by the average particle volume such that  $I(q) = \text{scale} \cdot \langle F^2 \rangle / \langle \text{Vol} \rangle + \text{bkg}$ , where  $F$  is the scattering amplitude of a sphere and the  $\langle \rangle$  denote an average over the size distribution. Resolution smeared version is also provided.

Additionally, two macros are provided to (1) calculate the number density based on the volume fraction and polydisperse particle volume (weighted using the 3rd moment of the

radius) and (2) plot the normalized probability distribution as a function of radius.

## VARIABLES

Input Variables (default values):

Point	parameters_bss	coef_bss
0	volume fraction(1)	0.01
1	Radius (1) (A)	200
2	polydispersity(1)	0.2
3	SLD(1) (A <sup>-2</sup> )	1e-06
4	volume fraction(2)	0.05
5	Radius (2)	25
6	polydispersity(2)	0.2
7	SLD(2)	1e-06
8	SLD (solvent)	6.4e-06
9	background (cm <sup>-1</sup> sr <sup>-1</sup> )	0.001

## USAGE NOTES

The returned value is scaled to units of [cm<sup>-1</sup> s r<sup>-1</sup>], absolute scale.

The subscripts (1) and (2) refer to the two populations. Each population has a Schulz distribution of radii, and the following description follows the documentation for the Schulz Spheres.

The (normalized) Schulz distribution is:

$$f(R) = (z + 1) \frac{\exp[-(z + 1)x]}{R_{avg} \Gamma(z + 1)}$$

where  $R_{avg}$  is the mean radius specified by W[1] above and  $x = R/R_{avg}$ ,  $z$  is related to the polydispersity,  $p = \sigma/R_{avg}$ , by  $z = 1/p^2 - 1$ .  $\sigma^2$  is the variance of the distribution. The distribution can be plotted for the radius and polydispersity in the coef\_bss wave using the macro "Plot\_Bimodal\_Distribution()".

The  $N^{th}$  moment of size distribution is equal to

$$\langle R^N \rangle = \frac{R_{avg}^N}{(z + 1)^N} \frac{(z + N)!}{z!}$$

The form factor is normalized by the average volume, using the 3<sup>rd</sup> moment of R:

$$\langle V \rangle = \frac{4\pi}{3} \langle R^3 \rangle = \frac{4\pi}{3} \langle R_{avg} \rangle^3 \frac{(z + 3)(z + 2)}{(z + 1)^2}$$

The variables w[0] and w[4] are the volume fraction of each of the populations, the total

volume fraction is the sum. Since there are two populations, there is no scale factor as in other models. The returned value is the differential macroscopic scattering cross-section (scattered cross-section per unit sample volume per unit solid angle).

$$I(q) = \left[ \left( \frac{4\pi}{3} \right)^2 N_1 \Delta\rho_1^2 \int_0^\infty f(R_1) R^6 F^2(qR_1) dR \right] + \left[ \left( \frac{4\pi}{3} \right)^2 N_2 \Delta\rho_2^2 \int_0^\infty f(R_2) R^6 F^2(qR_2) dR \right]$$

where  $N_0$  is the total number of particles per unit volume, and  $\Delta\rho = w[3]-w[8]$  or  $w[7] - w[8]$ , is the difference in scattering length density. The number of particles per unit volume having size between  $R$  and  $R+dR$  is equal to  $N(R)dR = N_0 f(R)dR$ . The Macro Plot\_Bimodal\_Distribution plots the function  $f(R)$  vs  $R$ .

The scattering amplitude for a sphere is

$$F(x) = \frac{[\sin(x) - x \cos(x)]}{x^3}$$

However, no interparticle interference effects are included in this calculation. Interparticle interference  $S(q)$  should be included by

$$I(q) = N_0 S(q) P(q)$$

where  $P(q)$  is the form factor. Some other relations of interest are:

$$N_0 = \phi / \langle V \rangle$$

Guinier radius:

$$R_G = \sqrt{\frac{3\langle R^8 \rangle}{5\langle R^6 \rangle}} = \sqrt{\frac{3(z+8)(z+7)}{5(z+1)^2}}$$

Total interfacial surface area per unit sample volume:

$$S_V = 4\pi \langle R^2 \rangle N_0 = \frac{3\phi}{R_{avg}} \frac{(z+1)}{(z+3)}$$

The forward scattering cross-section:

$$I(0) = N_0 \langle V^2 \rangle \Delta\rho^2$$

These values are calculated using the macro "NumberDensity\_Bimodal()" and use the current values in the coef\_bss wave.

$w[2]$  and  $w[6]$ (polydispersity ( $p$ )) must be between  $0 < p < 1$ .

NOTE that this calculation is an analytic solution and is much faster to compute than the Log Normal or Gaussian distributions of spheres which are both numerical solutions.

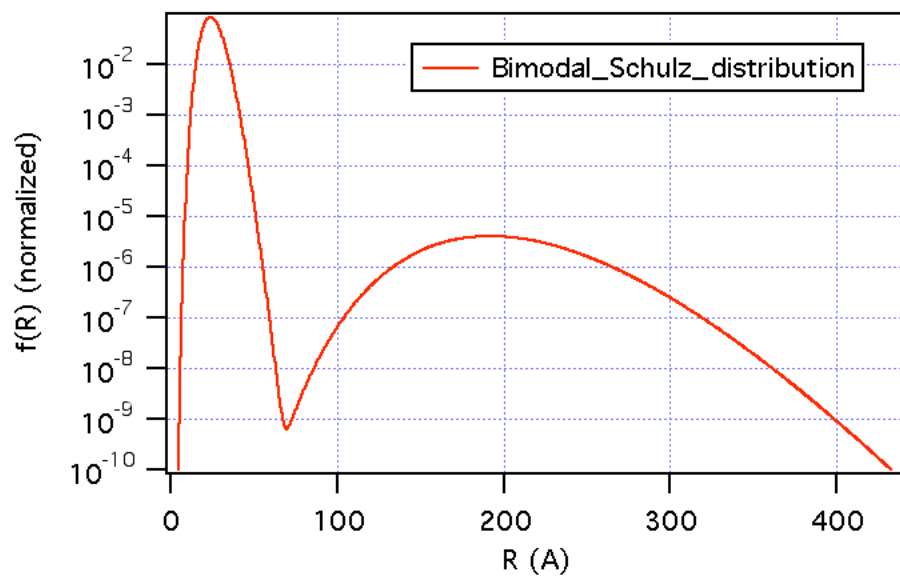
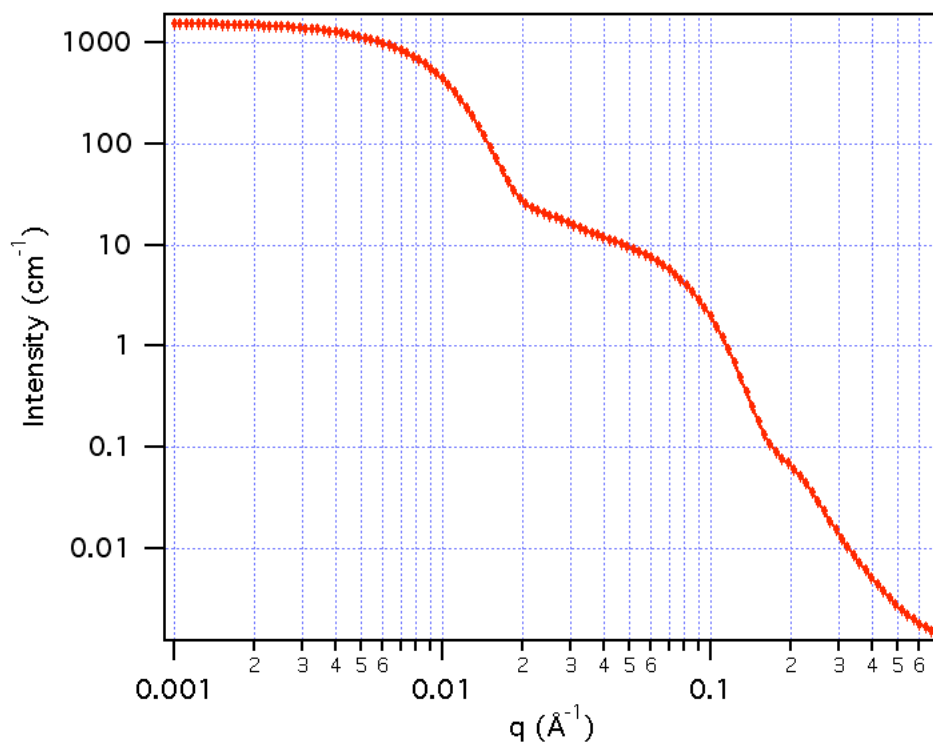
## REFERENCE

G. V. Schulz, *Z. Phys. Chem.*, **43** (1935) 25.

M. Kotlarchyk and S-H. Chen, *J. Chem. Phys.* **79** (1983) 2461-2469, eqn 25-29.

## TEST DATASET

This example dataset is produced by running the Macro PlotBimodalSchulzSpheres(), using 128 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_bss values.



(note the logarithmic Y-axis on the plot of the distribution)

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## **Monodisperse Rigid Cylinders**

### **MACRO : FUNCTION**

PlotCylinderForm() : CylinderForm(w,y,x)

Wave extension: \_cyl

File:

Cylinder.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

Function cyl(), included in CylinderForm.ipf

### **AUTHOR/MODIFICATION**

Steve Kline 06 NOV 1998

### **APPROVED FOR DISTRIBUTION**

Sungmin Choi 02 FEB 1999

### **DESCRIPTION**

Calculates the form factor for a monodisperse right circular cylinder with uniform scattering length density. The form factor is normalized by the particle volume such that  $P(q) = \text{scale} \cdot \langle f^2 \rangle / \text{Vol} + \text{bkg}$ , where  $\langle \rangle$  is an average over all possible orientations of the cylinder. Resolution smeared version is also provided.

### **VARIABLES**

Input Variables (default values):

parameters_cyl	coef_cyl
scale	1
radius (A)	20
length (A)	400
SLD cylinder (A <sup>-2</sup> )	1e-06
SLD solvent (A <sup>-2</sup> )	6.3e-06
incoh. bkg (cm <sup>-1</sup> )	0.01

### **USAGE NOTES**

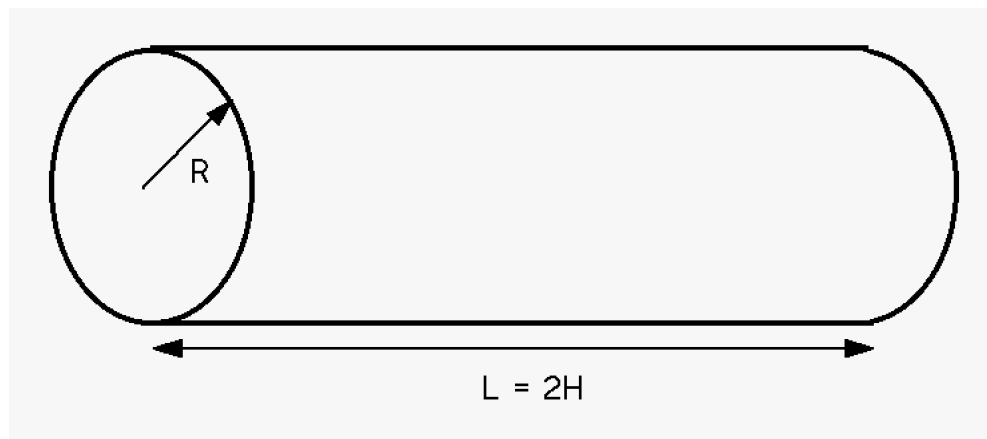
The function calculated is:

$$P(q) = \frac{\text{scale}}{V_{\text{cyl}}} \int_0^{\pi/2} f^2(q, \alpha) \sin \alpha d\alpha$$

$$f(q, \alpha) = 2(\rho_{\text{cyl}} - \rho_{\text{solv}}) V_{\text{cyl}} j_0(qH \cos \alpha) \frac{J_1(qr \sin \alpha)}{(qr \sin \alpha)}$$

$$V_{cyl} = \pi r^2 L \quad \text{and} \quad j_0(x) = \sin(x)/x$$

where  $J_1(x)$  is the first order Bessel function. Alpha is defined as the angle between the cylinder axis and the scattering vector,  $\mathbf{q}$ . The integral over alpha averages the form factor over all possible orientations of the cylinder with respect to  $\mathbf{q}$ . The returned value is in units of  $[\text{cm}^{-1}]$ , on absolute scale.



Scattering contrast ( $\Delta\rho$ ) = SLD (cylinder) - SLD (solvent)

The scale and scattering length densities (the contrast) are both multiplicative factors in the model and are perfectly correlated. One or both of these parameters must be held fixed during model fitting.

If the scale factor  $w[0]$  is set equal to the particle volume fraction,  $\phi$ , the returned value is the scattered intensity per unit volume,  $I(q) = \phi * P(q)$ . However, no interparticle interference effects are included in this calculation.

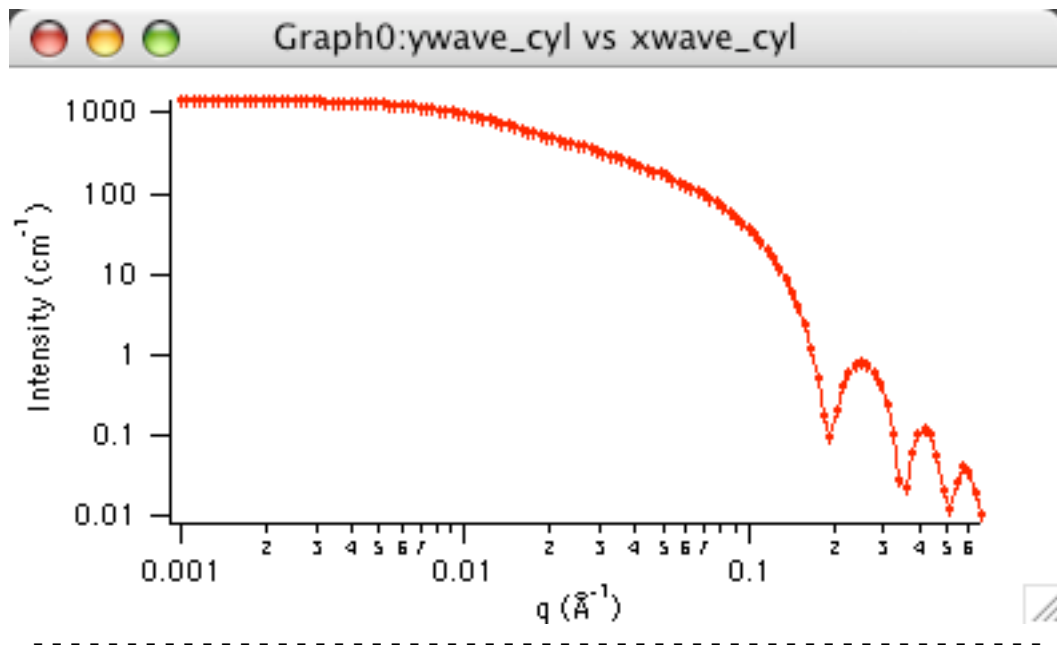
76-point Gaussian quadrature is used to calculate the form factor. This calculation will be slow (approximately 10 seconds) on older machines. The smearing calculation is an additional numerical integration (20-point quadrature) and will further slow the update of the graph.

## REFERENCE

Guinier, A. and G. Fournet, "Small-Angle Scattering of X-Rays", John Wiley and Sons, New York, (1955).

## TEST DATASET

This example dataset is produced by running the Macro PlotCylinderForm(), using 128 data points,  $q_{min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_cyl values.



### Cylinder with Elliptical Cross-Section

#### **MACRO : FUNCTION**

PlotEllipCylinderForm() : EllipCylForm(w,y,x)

Wave extension: \_ecf

File:

EllipticalCylinder.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

#### **AUTHOR/MODIFICATION**

Steve Kline 5 DEC 2000

#### **APPROVED FOR DISTRIBUTION**

Derek Ho 2 DEC 2003

#### **DESCRIPTION**

Calculates the form factor for a cylinder with uniform scattering length density and an elliptical cross section. The form factor is normalized by the particle volume such that  $P(q) = \text{scale} \cdot \langle f^2 \rangle / \text{Vol} + \text{bkg}$ , where  $\langle \rangle$  is an average over all possible orientations of the cylinder. An instrument resolution smeared version is also provided.

#### **VARIABLES**

Input Variables (default values):

parameters_ecf	coef_ecf
scale	1
minor radius (Å)	20
nu = major/minor (-)	1.5
length (Å)	400
SLD cylinder (Å <sup>-2</sup> )	1e-06
SLD solvent (Å <sup>-2</sup> )	6.3e-06
incoh. bkg (cm <sup>-1</sup> )	0

## USAGE NOTES

The function calculated is:

$$I(q) = scale \cdot \int_0^1 \Psi_{ec}[q, a(1-x^2)^{1/2}] S^2(qHx/2) dx + bkg$$

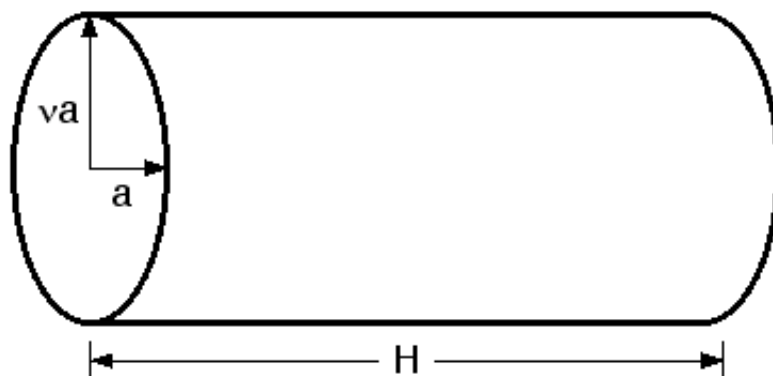
with the functions:

$$\Psi_{ec}(q, a) = \frac{1}{\pi} \int_0^\pi \Lambda_1^2 \left[ qa \left( \frac{1+v^2}{2} + \frac{1-v^2}{2} \cos(y) \right)^{1/2} \right] dy$$

$$\Lambda_1 = 2J_1(t)/t$$

and  $J_1(x)$  is the first order Bessel function. The returned value is in units of [cm<sup>-1</sup>], on absolute scale. The elliptical cylinder is as depicted in the figure, with a total length  $H$ , minor radius  $a$ , and major radius  $va$ . The ellipticity (parameter 2) is defined as:

$$v = R_{\text{major}} / R_{\text{minor}} \geq 1$$



The volume and radius of gyration of the cylinder is given by:

$$V = \pi v a^2 H$$



$$R_g^2 = \frac{a^2 + b^2}{4} + \frac{H^2}{12}$$

Scattering contrast ( $\Delta\rho$ ) = SLD (cylinder) - SLD (solvent)

w[0] (scale) and contrast are both multiplicative factors in the model and are perfectly correlated. One or both of these parameters must be held fixed during model fitting.

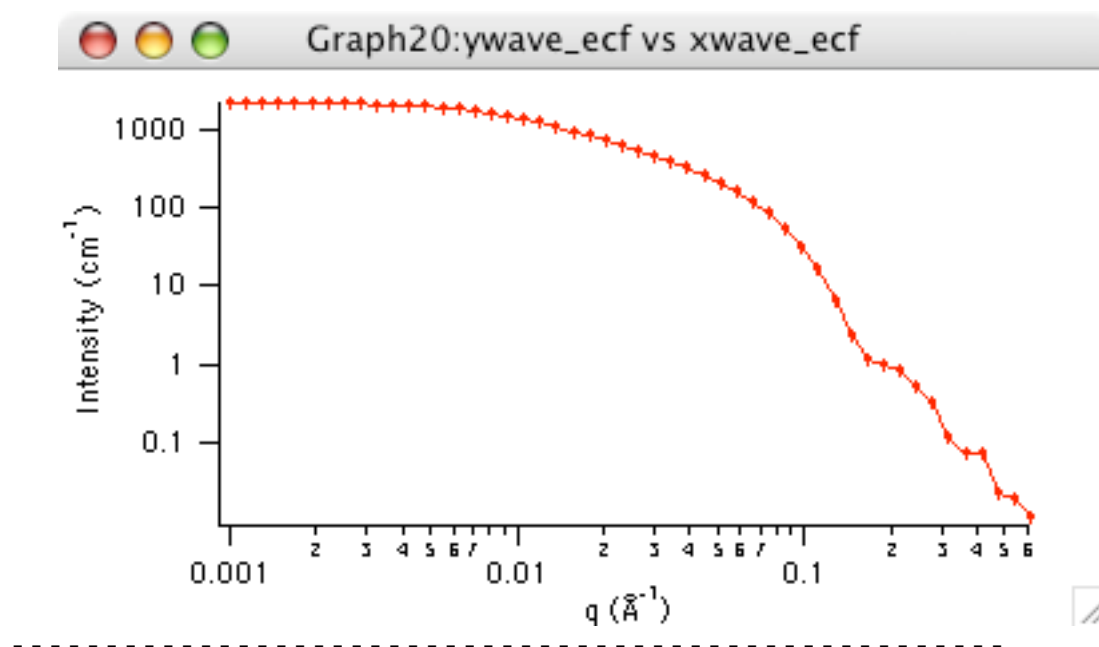
If the scale factor w[0] is set equal to the particle volume fraction,  $\phi$ , the returned value is the scattered intensity per unit volume,  $I(q) = \phi * P(q)$ . However, no interparticle interference effects are included in this calculation.

## REFERENCE

L. A. Feigin and D. I. Svergun "Structure Analysis by Small-Angle X-Ray and Neutron Scattering", Plenum, New York, 1987.

## TEST DATASET

This example dataset is produced by running the Macro PlotEllipCylinderForm(), using 50 data points,  $q_{min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_ecf values.



## Core-Shell Cylinder

### MACRO : FUNCTION

PlotCoreShellCylinderForm() : CoreShellCylinderForm(w,y,x)

Wave extension: \_cscyl

File:

CoreShellCylinder.ipf

Requires:

## AUTHOR/MODIFICATION

Steve Kline 20 JAN 1999

## APPROVED FOR DISTRIBUTION

Sungmin Choi 02 FEB 1999

## DESCRIPTION

Calculates the form factor for a monodisperse, right circular cylinder with a core-shell scattering length density profile. The shell thickness,  $t$ , is considered to be uniform over the entire surface of the core. The form factor is normalized by the total particle volume such that  $P(q) = \text{scale} \cdot \langle f^2 \rangle / \text{Vol} + \text{bkg}$ , where  $f$  is the scattering amplitude and the  $\langle \rangle$  denote an average over all possible orientations of the cylinder. Resolution smeared version is also provided.

## VARIABLES

Input Variables (default values):

Point	parameters_cscyl	coef_cscyl
0	scale	1
1	core radius (A)	20
2	shell THICKNESS (A)	10
3	CORE length (A)	400
4	SLD core (A <sup>-2</sup> )	1e-06
5	SLD shell (A <sup>-2</sup> )	4e-06
6	SLD solvent (A <sup>-2</sup> )	1e-06
7	incoh. bkg (cm <sup>-1</sup> )	0.001

## USAGE NOTES

The function calculated is:

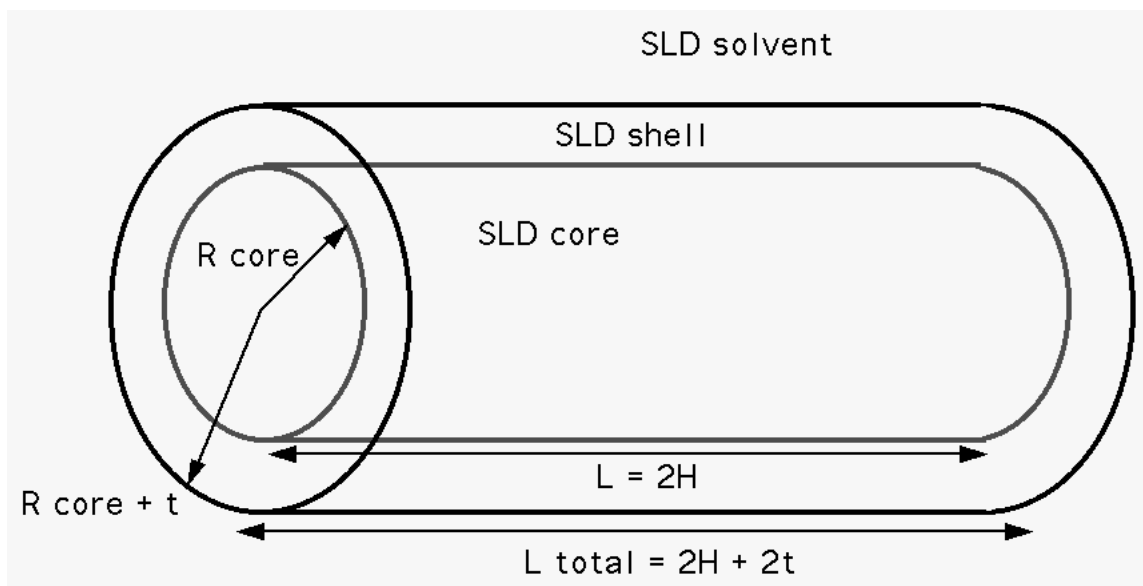
$$P(q) = \frac{\text{scale}}{V_{\text{shell}}} \int_0^{\pi/2} f^2(q, \alpha) \sin \alpha d\alpha$$

$$f(q, \alpha) = 2(\rho_{\text{core}} - \rho_{\text{shell}}) V_{\text{core}} j_0(qH \cos \alpha) \frac{J_1(qr \sin \alpha)}{(qr \sin \alpha)} \\ + 2(\rho_{\text{shell}} - \rho_{\text{solvent}}) V_{\text{shell}} j_0[q(H+t) \cos \alpha] \frac{J_1[q(r+t) \sin \alpha]}{[q(r+t) \sin \alpha]}$$

$$j_0(x) = \sin(x)/x, \quad V_{\text{core}} = \pi r^2 L \quad \text{and} \quad V_{\text{shell}} = \pi(r+t)^2 L_{\text{total}}$$

where  $r$  is the radius of the core of the cylinder as shown below, and  $J_1(x)$  is the first order bessel function. Alpha is defined as the angle between the cylinder axis and the scattering vector,  $q$ . The integral over alpha averages the form factor over all possible

orientations of the cylinder. The returned value is scaled to units of  $[\text{cm}^{-1}]$ , on absolute scale.



The shell thickness is uniform over the entire particle. This means that for the default case above, the total *diameter* of the cylinder is  $2 \times 20 + 2 \times 10 = 60$  Å and that the total *length* is  $400 + 2 \times 10 = 420$  Å. The calculated cylinder volume is based on these total cylinder dimensions.

The contrasts in the default case correspond to scattering from a cylindrical shell.

$w[0]$  (scale) and  $w[4]$ ,  $w[5]$ , and  $w[6]$  (SLD's) are multiplicative factors in the model and are perfectly correlated. Only one of these four parameters should be left free during model fitting.

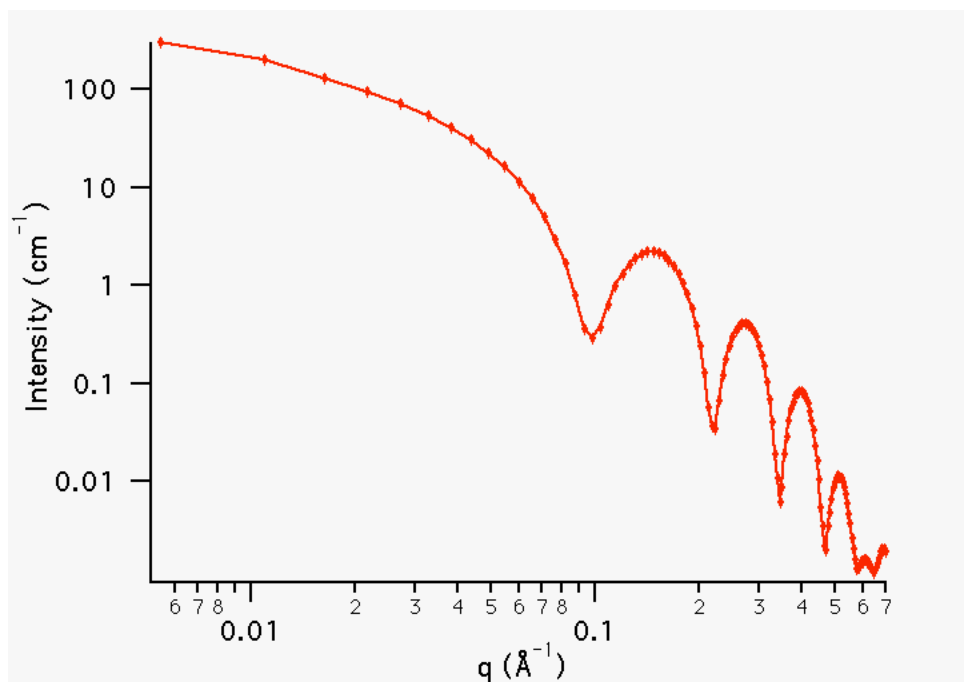
If the scale factor  $w[0]$  is set equal to the particle volume fraction,  $\phi$ , the returned value is the scattered intensity per unit volume,  $I(q) = \phi \cdot P(q)$ . However, no interparticle interference effects are included in this calculation.

## REFERENCE

I. Livsey, J. Chem. Soc. Faraday Trans. 2 (1987) 83(8) 1445-1452. Equation (3).

## TEST DATASET

This example dataset is produced by running the Macro PlotCoreShellCylinderForm(), using 128 data points,  $q_{\min} = 0.001 \text{ Å}^{-1}$ ,  $q_{\max} = 0.7 \text{ Å}^{-1}$  and the above default coef\_cscyl values.



## Hollow Cylinder

### MACRO : FUNCTION

PlotHollowCylinderForm() : HollowCylinderForm(w,y,x)

Wave extension: \_Hcyl

File:

HollowCylinders.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

### AUTHOR/MODIFICATION

Steve Kline 20 JAN 1999

### APPROVED FOR DISTRIBUTION

Sungmin Choi 02 FEB 1999

### DESCRIPTION

Calculates the form factor for a monodisperse, hollow, right circular cylinder (or a tube). The inside and outside of the tube have the same scattering length density and the tube itself is of uniform SLD. The form factor is normalized by the tube material volume ONLY such that  $P(q) = \text{scale} \cdot \langle f^2 \rangle / \text{Vol} + \text{bkg}$ , where  $f$  is the scattering amplitude and the  $\langle \rangle$  denote an average over all possible orientations of the cylinder. Resolution smeared version is also provided.

### VARIABLES

Input Variables (default values):

parameters_Hcyl	coef_Hcyl
scale	1
core radius (A)	20
shell radius (A)	30
length (A)	400
SLD shell (A <sup>-2</sup> )	1e-06
SLD solvent (in/out)	6.3e-06
incoh. bkg (cm <sup>-1</sup> )	0.01

## USAGE NOTES

The function calculated is:

$$P(q) = scale \cdot V_{shell} \cdot (\Delta\rho)^2 \int_0^1 \Psi^2[q, R_{shell}(1-x^2)^{1/2}, R_{core}(1-x^2)^{1/2}] \left( \frac{\sin(qHx)}{qHx} \right)^2 dx$$

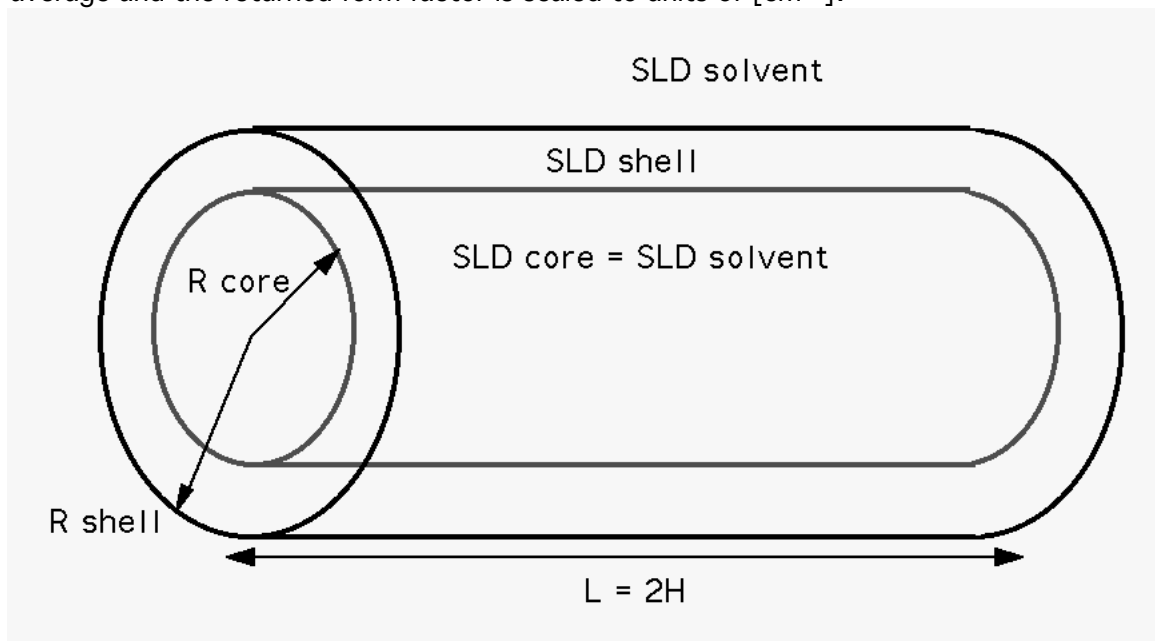
$$\Psi(q, y, z) = \frac{1}{1-\gamma^2} [\Lambda(qy) - \gamma^2 \Lambda(qz)]$$

$$\Lambda(w) = 2J_1(w) / w$$

$$\gamma = R_{core} / R_{shell}$$

$$V_{shell} = \pi(R_{shell}^2 - R_{core}^2)L$$

where  $J_1$  is the first order Bessel function. The integral over  $x$  is the orientational average and the returned form factor is scaled to units of  $[\text{cm}^{-1}]$ .



$$\text{contrast} = \text{SLD (shell)} - \text{SLD (solvent)}$$

The shell thickness is uniform over the cylinder radius. There is no material covering the ends of the tube. This means that for the default case above, the total *diameter* of the cylinder is  $2 \times 30 = 60$  A and that the total *length* is 400 A. The 40 A diameter core is assumed to be the same scattering length density as the solvent, giving no contribution to the scattered intensity.

The form factor is normalized to the volume of material comprising the shell such that  $V_{shell} = \pi(R_{shell}^2 - R_{core}^2)L$ . Note that this is different than the total excluded volume of the hollow cylinder, which is  $V_{excl} = \pi R_{shell}^2 L$ .

w[0] (scale) and w[4] (contrast) are multiplicative factors in the model and are perfectly correlated. Only one of these parameters should be left free during model fitting.

The user should ensure that the shell radius is always larger than the core radius.

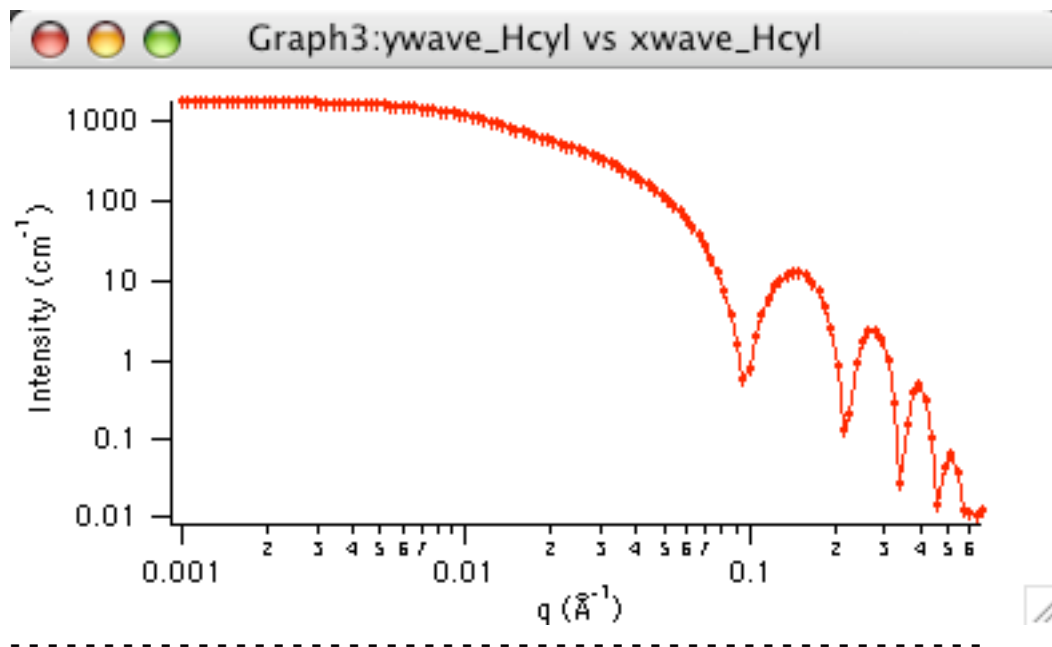
If the scale factor w[0] is set equal to the particle volume fraction,  $\phi$ , the returned value is the scattered intensity per unit volume,  $I(q) = \phi * P(q)$ . However, no interparticle interference effects are included in this calculation.

## REFERENCE

Feigin, L. A, and D. I. Svergun, "Structure Analysis by Small-Angle X-Ray and Neutron Scattering", Plenum Press, New York, (1987).

## TEST DATASET

This example dataset is produced by running the Macro PlotHollowCylinderForm(), using 128 data points,  $q_{min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_Hcyl values.



## Cylinder - Polydisperse Length

### MACRO : FUNCTION

PlotCyl\_PolyLength() : Cyl\_PolyLength(w,y,x)

Wave extension: \_cyl

File:

## Cylinder\_PolyLength.ipf

Requires:

GaussUtils.ipf  
PlotUtils.ipf  
[CylinderForm.ipf](#)

### **AUTHOR/MODIFICATION**

Steve Kline 5 DEC 2000

### **APPROVED FOR DISTRIBUTION**

Derek Ho 2 DEC 2003

### **DESCRIPTION**

Calculates the form factor for a polydisperse right circular cylinder with uniform scattering length density. A Schulz polydispersity of the cylinder length is considered. The form factor is normalized by the particle volume such that  $P(q) = \text{scale} \cdot \langle f^2 \rangle / \text{Vol} + \text{bkg}$ , where  $\langle \rangle$  is an average over all possible orientations of the cylinder. The form factor is then averaged over the normalized size distribution. An instrument resolution smeared version is also provided.

### **VARIABLES**

Input Variables (default values):

parameters_cypl	coef_cypl
scale	1
radius (A)	20
length (A)	1000
polydispersity of Length	0.2
SLD cylinder (A <sup>-2</sup> )	1e-06
SLD solvent (A <sup>-2</sup> )	6.3e-06
incoh. bkg (cm <sup>-1</sup> )	0.01

### **USAGE NOTES**

The function calculated is the orientationally averaged cylinder form factor which is then averaged over a Schulz distribution of the cylinder length. See the documentation for the cylinder form factor for details of the monodisperse calculation. The polydispersity is included by integrating the form factor over a Schulz distribution of cylinder length. The integration has been normalized by the first moment of the length distribution. This insures that the invariant is constant when the polydispersity is varied and all other structural parameters are held fixed.

Polydispersity of the cylinder length usually has little effect on the scattered intensity, and is only (weakly) visible at low enough q-values that correspond to the average cylinder length.

The size averaged form factor is thus:

$$\overline{P(q)} = \frac{1}{V_{poly}} \int_0^x P(q) f(r) dr$$

where  $f(r)$  is the normalized Schulz distribution of the length. The limits of the integration are chosen automatically to cover the full range of length. The calculation is normalized to the polydisperse volume using the first moment.

See the Schulz Spheres documentation for the definition of the Schulz distribution and associated moments.

$P(q)$  is the orientation-averaged form factor of a cylinder of total length  $H$  and radius  $r$ :

$$P(q) = \frac{scale}{V_{cyl}} \int_0^{\pi/2} F^2(q, \alpha) \sin \alpha d\alpha$$

where the scattering amplitude is:

$$F(q, \alpha) = 2 V_{cyl} (\rho_{cyl} - \rho_{solv}) j_0(qH \cos \alpha) \frac{J_1(qr \sin \alpha)}{(qr \sin \alpha)}$$

See the documentation for the cylinder form factor for the definition of the angles and details of the monodisperse calculation.

Scattering contrast ( $\Delta\rho$ ) = SLD (cylinder) - SLD (solvent)

$w[0]$  (scale) and contrast are both multiplicative factors in the model and are perfectly correlated. One or both of these parameters must be held fixed during model fitting.

If the scale factor  $w[0]$  is set equal to the particle volume fraction,  $\phi$ , the returned value is the scattered intensity per unit volume,  $I(q) = \phi * P(q)$ . However, no interparticle interference effects are included in this calculation.

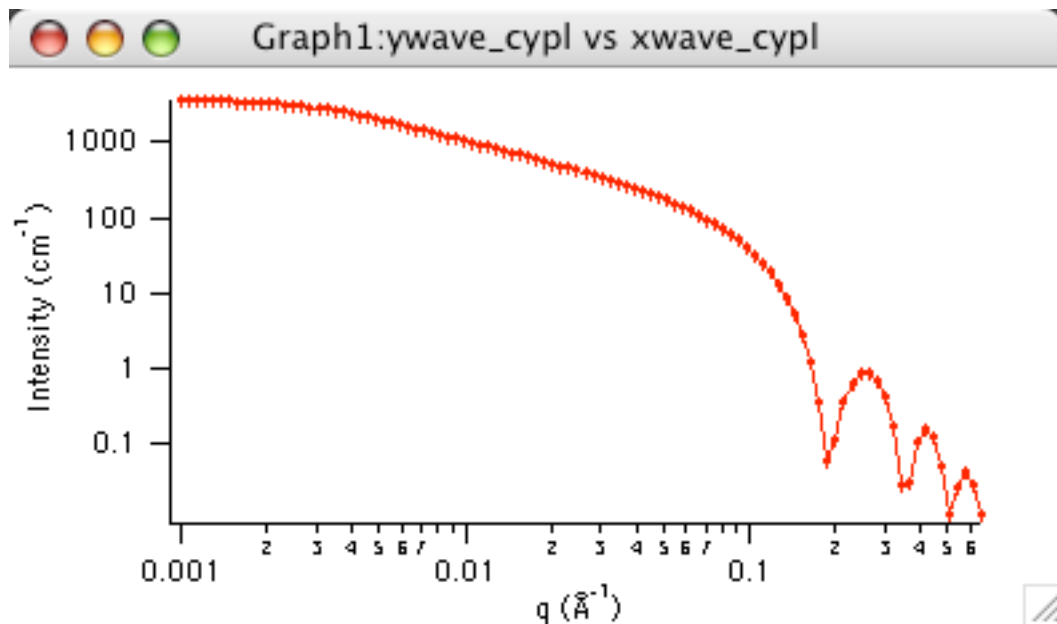
## REFERENCE

Guinier, A. and G. Fournet, "Small-Angle Scattering of X-Rays", John Wiley and Sons, New York, (1955).

## TEST DATASET

This example dataset is produced by running the Macro `PlotCyl_PolyLength()`, using 100 data points,  $q_{min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{max} = 0.7 \text{ \AA}^{-1}$  and the above default `coef_cyl` values.





### Cylinder - Polydisperse Radius

#### **MACRO : FUNCTION**

PlotCyl\_PolyRadius() : Cyl\_PolyRadius(w,y,x)

Wave extension: \_cypr

File:

Cylinder\_PolyRadius.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

[CylinderForm.ipf](#)

#### **AUTHOR/MODIFICATION**

Steve Kline 5 DEC 2000

#### **APPROVED FOR DISTRIBUTION**

Derek Ho 2 DEC 2003

#### **DESCRIPTION**

Calculates the form factor for a polydisperse right circular cylinder with uniform scattering length density. A Schulz polydispersity of the cylinder radius is considered. The form factor is normalized by the particle volume such that  $P(q) = \text{scale} \cdot \langle f^2 \rangle / \text{Vol} + \text{bkg}$ , where  $\langle \rangle$  is an average over all possible orientations of the cylinder. The form factor is then averaged over the normalized size distribution. An instrument resolution smeared version is also provided.

#### **VARIABLES**

Input Variables (default values):

parameters_cypr	coef_cypr
scale	1
radius (Å)	20
length (Å)	400
polydispersity of Radius	0.2
SLD cylinder (Å <sup>-2</sup> )	1e-06
SLD solvent (Å <sup>-2</sup> )	6.3e-06
incoh. bkg (cm <sup>-1</sup> )	0.01

## USAGE NOTES

The function calculated is the orientationally averaged cylinder form factor which is then averaged over a Schulz distribution of the cylinder radius. The polydispersity is included by integrating the form factor,  $P(q)$ , over a Schulz distribution of cylinder radius. The integration has been normalized by the second moment of the radius distribution. This insures that the invariant is constant when the polydispersity is varied and all other structural parameters are held fixed. The size averaged form factor is thus:

$$\overline{P(q)} = \frac{1}{V_{poly}} \int_0^x P(q) f(r) dr$$

where  $f(r)$  is the normalized Schulz distribution of the radius. The limits of the integration are chosen automatically to cover the full range of radius. The calculation is normalized to the polydisperse volume using the second moment:

$$V_{poly} = \pi r^2 L \left( \frac{z+2}{z+1} \right)$$

See the Schulz Spheres documentation for the definition of the Schulz distribution and associated moments.

$P(q)$  is the orientation-averaged form factor of a cylinder of total length  $H$  and radius  $r$ :

$$P(q) = \frac{scale}{V_{cyl}} \int_0^{\pi/2} F^2(q, \alpha) \sin \alpha d\alpha$$

where the scattering amplitude is:

$$F(q, \alpha) = 2 V_{cyl} (\rho_{cyl} - \rho_{solv}) j_0(qH \cos \alpha) \frac{J_1(qr \sin \alpha)}{(qr \sin \alpha)}$$

See the documentation for the cylinder form factor for the definition of the angles and details of the monodisperse calculation.

Scattering contrast ( $\Delta\rho$ ) = SLD (cylinder) - SLD (solvent)

w[0] (scale) and contrast are both multiplicative factors in the model and are perfectly correlated. One or both of these parameters must be held fixed during model fitting.

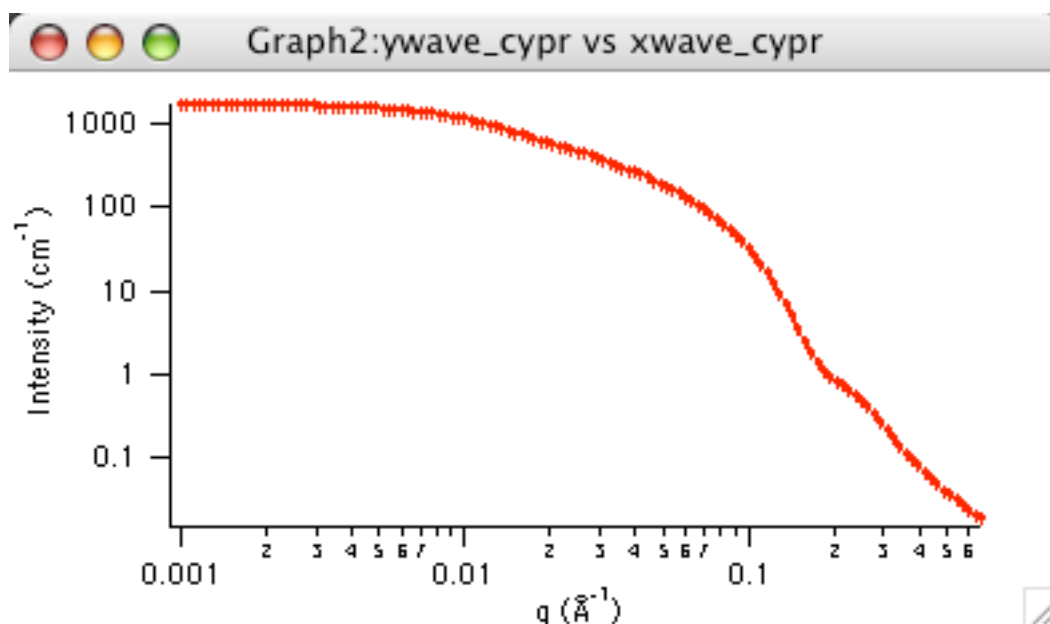
If the scale factor w[0] is set equal to the particle volume fraction,  $\phi$ , the returned value is the scattered intensity per unit volume,  $I(q) = \phi * P(q)$ . However, no interparticle interference effects are included in this calculation.

## REFERENCE

Guinier, A. and G. Fournet, "Small-Angle Scattering of X-Rays", John Wiley and Sons, New York, (1955).

## TEST DATASET

This example dataset is produced by running the Macro PlotCyl\_PolyRadius(), using 128 data points,  $q_{min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_cypr values.



## Core-Shell Cylinder - Polydisperse Radius

### MACRO : FUNCTION

PlotPolyCoShCylinder() : PolyCoShCylinder(w,y,x)

Wave extension : \_CSCpr

File:

[PolyCoreShellCylinder.ipf](#)

Requires:

GaussUtils.ipf

PlotUtils.ipf

## AUTHOR/MODIFICATION

Andrew Nelson 27 APR 2003

## APPROVED FOR DISTRIBUTION

WeiRen Chen 01 FEB 2006

## DESCRIPTION

This function calculates the scattering for a polydisperse, right circular cylinder with a core-shell scattering length density profile. The shell thickness on the flat ends of the cylinder is independent of the shell thickness on the radial surface. Polydispersity of the cylinder core radius is modelled using a log-normal distribution. The overall intensity is obtained by calculating the scattering from each particle size present and weighting it by the normalised distribution.

## VARIABLES

Input variables (default values):

Point	parameters_CSCpr	coef_CSCpr
0	scale	0.01
1	mean CORE radius (A)	150
2	radial polydispersity (sigma)	0.1
3	CORE length (A)	10
4	radial shell thickness (A)	20
5	face shell thickness (A)	10
6	SLD core (A <sup>-2</sup> )	4e-06
7	SLD shell (A <sup>-2</sup> )	1e-06
8	SLD solvent (A <sup>-2</sup> )	4e-06
9	incoh. bkg (cm <sup>-1</sup> )	0.001

## USAGE NOTES

The function calculated is:

$$I(Q) = bkg + \frac{scale}{V_p} \sum_{R_p} n(R_p, \sigma_p) P(Q, R_p, R_l, H_p, H_l, \rho_p, \rho_l, \rho_{solv})$$

with the normalised log-normal distribution:

$$n(R_p) = \frac{\exp\left(-\frac{1}{2}\left[\frac{\ln(R_p/R_o)}{\sigma_p}\right]^2\right)}{\sqrt{(2\pi)}\sigma_p R_p}$$

and

$$P(Q) = \int_0^{\pi/2} \sin\theta \cdot d\theta \cdot \left[ V_l(\rho_l - \rho_{solv}) \frac{\sin\left(\frac{QH_l \cos\theta}{2}\right)}{\frac{QH_l \cos\theta}{2}} \frac{2J_1(QR_l \sin\theta)}{QR_l \sin\theta} + V_p(\rho_p - \rho_l) \frac{\sin\left(\frac{QH_p \cos\theta}{2}\right)}{\frac{QH_p \cos\theta}{2}} \frac{2J_1(QR_p \sin\theta)}{QR_p \sin\theta} \right]^2$$

$$V_x = \pi R_x^2 H_x$$

$J_1(x)$  is the first order Bessel function. Theta is defined as the angle between the cylinder axis and the scattering vector, Q. The integral over theta averages the form factor over all possible orientations of the cylinder with respect to Q. The core radius =  $R_p$ , core length =  $H_p$  (the mean core radius is  $R_0$ ). Note that the shell radius and shell length incorporate the dimensions of the bare particle (i.e  $H_l = H_p + 2 \cdot \text{face thickness}$  and  $R_l = R_p + \text{radial thickness}$ ). Sigma is equivalent to the standard deviation of the log-normal distribution.

The form factor  $P(Q)$  is normalised by multiplying by  $\text{scale}/V_p$ . If scale represents the volume fraction of the core particles then the multiplication factor is the number density of particles and an absolute intensity is returned.

Note that the shell has a constant thickness around the edge of the particle.

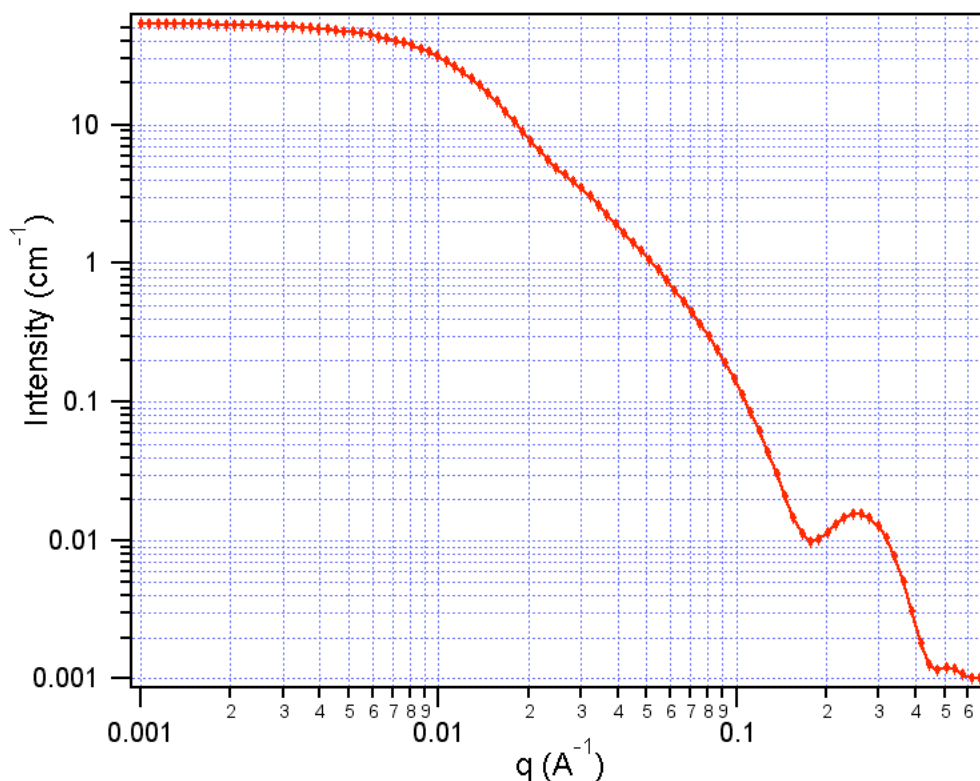
76-point Gaussian quadrature is used to calculate the form factor and 20-point Gaussian quadrature is used to integrate the polydispersity. The fitting procedure is likely to run very slowly on old machines.

## REFERENCE

Guinier, A.; Fournet, G. "Small-Angle Scattering of X-Rays"; 1 ed.; Wiley: New York, 1955.

## TEST DATASET

This example dataset is produced by running the Macro `PlotPolyCoShCylinder()`, using 100 data points,  $Q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $Q_{\max} = 0.7 \text{ \AA}^{-1}$  and the above default `coef_CSCpr` values.



## Monodisperse Flexible Cylinders

### MACRO : FUNCTION

PlotFlexExclVolCyl() : FlexExclVolCyl(w,y,x)

Wave extension : \_fle

File:

FlexibleCylinder.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

### AUTHOR/MODIFICATION

Wei-Ren Chen 1 JUL 2006

### APPROVED FOR DISTRIBUTION

Steve Kline 15 JUL 2006

### DESCRIPTION

Calculates the form factor for a flexible cylinder with a circular cross section and a uniform scattering length density. The non-negligible diameter of the cylinder is included by accounting for excluded volume interactions within the walk of a single cylinder. Inter-cylinder interactions are NOT included. The form factor is normalized by the particle volume such that  $P(q) = \text{scale} \cdot \langle f^2 \rangle / \text{Vol} + \text{bkg}$ , where  $\langle \rangle$  is an average over all possible orientations of the flexible cylinder. An instrument resolution smeared version is also provided.

### VARIABLES

Input Variables (default values):

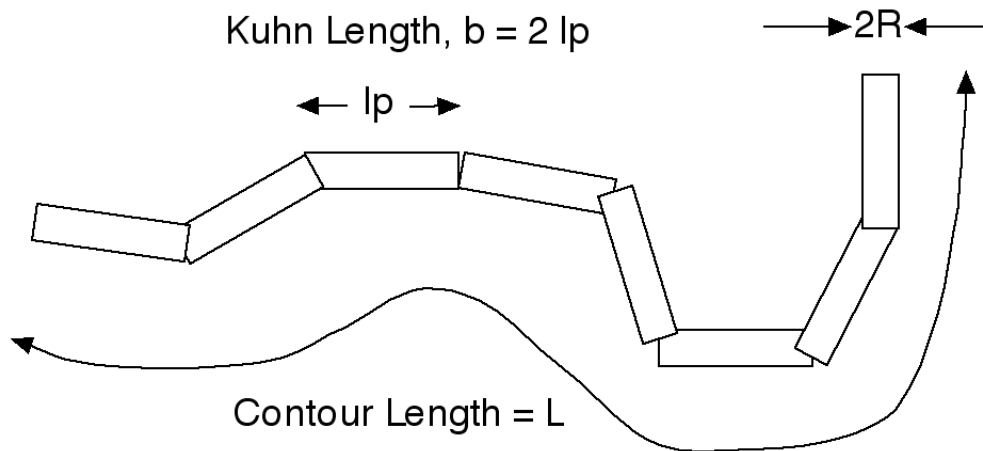
parameters_fle	coef_fle
scale	1
Contour Length (A)	1000
Kuhn Length, b (A)	100
Radius (A)	20
SLD cylinder (A <sup>-2</sup> )	1e-06
SLD solvent (A <sup>-2</sup> )	6.3e-06
bkgd (cm <sup>-1</sup> )	0.0001

## USAGE NOTES

The function calculated is from the reference given below. From that paper, "Method 3 With Excluded Volume" is used. The model is a parametrization of simulations of a discrete representation of the worm-like chain model of Kratky and Porod applied in the pseudocontinuous limit. See equations (13,26-27) in the original reference for the details.

**NOTE:** there are several typos in the original reference that have been corrected by WRC. Details of the corrections are in the reference below.

- Equation (13): the term  $(1-w(QR))$  should swap position with  $w(QR)$
- Equations (23) and (24) are incorrect. WRC has entered these into Mathematica and solved analytically. The results were converted to code.
- Equation (27) should be  $q_0 = \max(a_3/\sqrt{R_g^2}, 3)$  instead of  $\max(a_3*b/\sqrt{R_g^2}, 3)$
- The scattering function is negative for a range of parameter values and q-values that are experimentally accessible. A correction function has been added to give the proper behavior.



The chain of contour length,  $L$ , (the total length) can be described a chain of some number of locally stiff segments of length  $l_p$ . The persistence length,  $l_p$ , is the length along the cylinder over which the flexible cylinder can be considered a rigid rod. the Kuhn length ( $b$ ) used in the model is also used to describe the stiffness of a chain, and is simply  $b = 2 * l_p$ .

The returned value is in units of  $[\text{cm}^{-1}]$ , on absolute scale.

Scattering contrast ( $\Delta\rho$ ) = SLD (chain) - SLD (solvent)

$w[0]$  (scale) and contrast are both multiplicative factors in the model and are perfectly correlated. One or both of these parameters must be held fixed during model fitting.

If the scale factor  $w[0]$  is set equal to the particle volume fraction,  $\phi$ , the returned value is the scattered intensity per unit volume,  $I(q) = \phi * P(q)$ . However, no interparticle interference effects are included in this calculation.

## REFERENCE

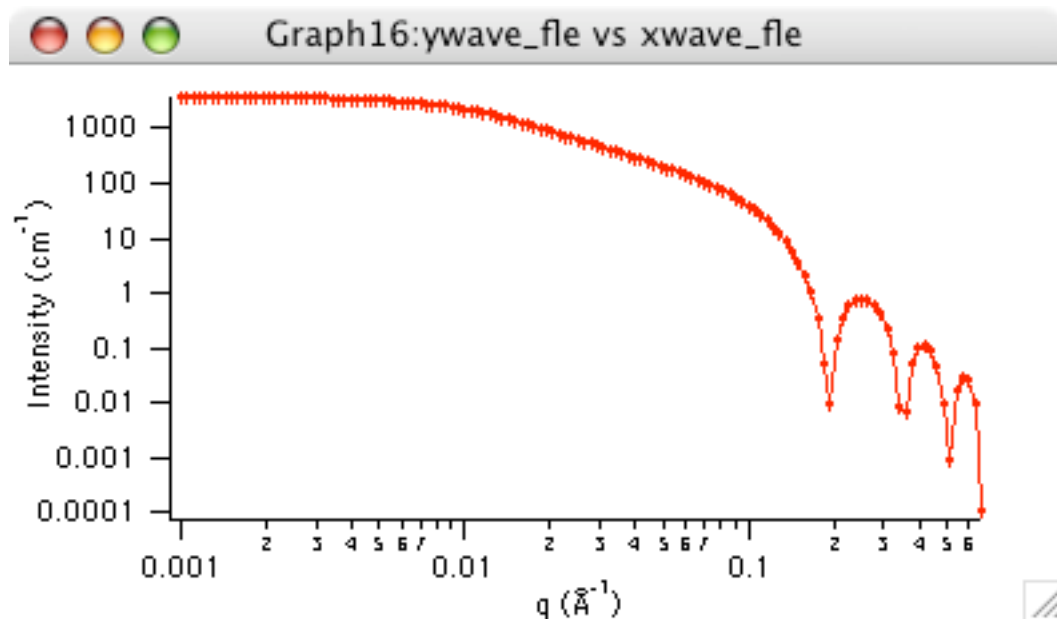
Pedersen, J. S. and P. Schurtenberger (1996). "Scattering functions of semiflexible polymers with and without excluded volume effects." *Macromolecules* 29: 7602-7612.

Corrections are in:

Wei-Ren Chen, Paul D. Butler, and Linda J. Magid, "Incorporating Intermicellar Interactions in the Fitting of SANS Data from Cationic Wormlike Micelles" *Langmuir*, August 2006.

## TEST DATASET

This example dataset is produced by running the Macro PlotFlexExclVolCyl(), using 128 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_fle values.



Flexible Cylinder with Elliptical Cross-Section



**MACRO : FUNCTION**

PlotFlexCyl\_Ellip() : FlexCyl\_Ellip(w,y,x)

Wave extension : \_fleell

File:

FlexCyl\_EllipCross.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

**AUTHOR/MODIFICATION**

Wei-Ren Chen 1 JUL 2006

**APPROVED FOR DISTRIBUTION**

Steve Kline 15 JUL 2006

**DESCRIPTION**

Calculates the form factor for a flexible cylinder with an elliptical cross section and a uniform scattering length density. The non-negligible diameter of the cylinder is included by accounting for excluded volume interactions within the walk of a single cylinder. Inter-cylinder interactions are NOT included. The form factor is normalized by the particle volume such that  $P(q) = \text{scale} \cdot \langle f^2 \rangle / \text{Vol} + \text{bkg}$ , where  $\langle \rangle$  is an average over all possible orientations of the flexible cylinder. An instrument resolution smeared version is also provided.

**VARIABLES**

Input Variables (default values):

parameters_fleell	coef_fleell
scale	1
Contour Length (A)	1000
Kuhn Length, b (A)	100
Minor Radius (a) (A)	20
Axis Ratio = major/a	1.5
SLD cylinder (A <sup>-2</sup> )	1e-06
SLD solvent (A <sup>-2</sup> )	6.3e-06
bkgd (arb)	0.0001

**USAGE NOTES**

The function calculated is from the reference given below. From that paper, "Method 3 With Excluded Volume" is used. The model is a parametrization of simulations of a discrete representation of the worm-like chain model of Kratky and Porod applied in the pseudocontinuous limit. See equations (13,26-27) in the original reference for the details.

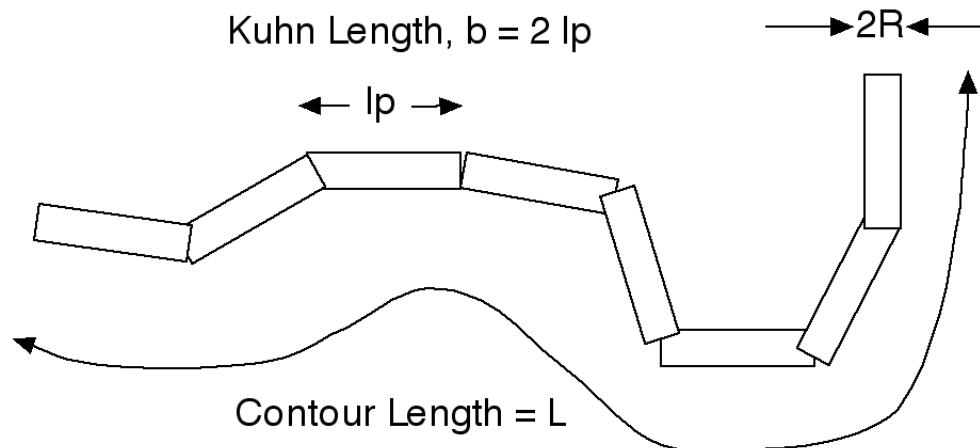
**NOTE:** there are several typos in the original reference that have been corrected by WRC. Details of the corrections are in the reference below.

- Equation (13): the term (1-w(QR)) should swap position with w(QR)
- Equations (23) and (24) are incorrect. WRC has entered these into Mathematica and

solved analytically. The results were converted to code.

- Equation (27) should be  $q_0 = \max(a^3/\sqrt{R_g^2}, 3)$  instead of  $\max(a^3*b/\sqrt{R_g^2}, 3)$

- The scattering function is negative for a range of parameter values and q-values that are experimentally accessible. A correction function has been added to give the proper behavior.



The chain of contour length,  $L$ , (the total length) can be described a chain of some number of locally stiff segments of length  $l_p$ . The persistence length,  $l_p$ , is the length along the cylinder over which the flexible cylinder can be considered a rigid rod. the Kuhn length ( $b$ ) used in the model is also used to describe the stiffness of a chain, and is simply  $b = 2 * l_p$ .

The cross section of the cylidner is elliptical, with minor radius  $a$ . The major radius is larger, so of course, the axis ratio (parameter 4) must be greater than one. Simple constraints should be applied during curve fitting to maintain this inequality.

The returned value is in units of  $[\text{cm}^{-1}]$ , on absolute scale.

Scattering contrast ( $\Delta\rho$ ) = SLD (chain) - SLD (solvent)

$w[0]$  (scale) and contrast are both multiplicative factors in the model and are perfectly correlated. One or both of these parameters must be held fixed during model fitting.

If the scale factor  $w[0]$  is set equal to the particle volume fraction,  $\phi$ , the returned value is the scattered intensity per unit volume,  $I(q) = \phi * P(q)$ . However, no interparticle interference effects are included in this calculation.

## REFERENCE

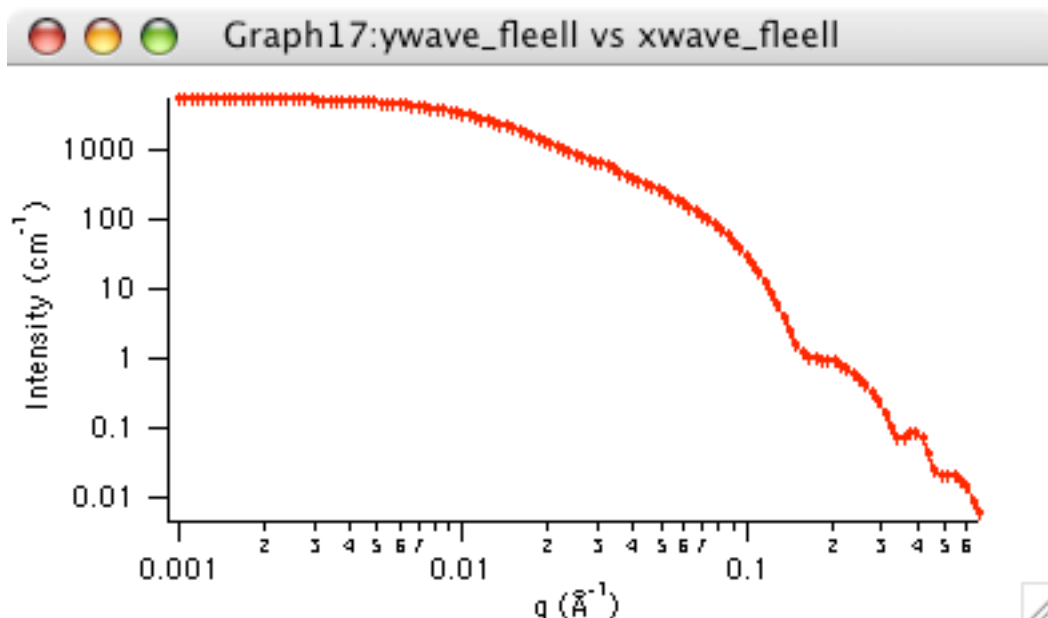
Pedersen, J. S. and P. Schurtenberger (1996). "Scattering functions of semiflexible polymers with and without excluded volume effects." *Macromolecules* 29: 7602-7612.

Corrections are in:

Wei-Ren Chen, Paul D. Butler, and Linda J. Magid, "Incorporating Intermicellar Interactions in the Fitting of SANS Data from Cationic Wormlike Micelles" *Langmuir*, August 2006.

## TEST DATASET

This example dataset is produced by running the Macro PlotFlexCyl\_Ellip(), using 128 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_fleell values.



## Flexible Cylinder - Polydisperse Length

### MACRO : FUNCTION

PlotFlexCyl\_PolyLength() : FlexCyl\_PolyLen(w,y,x)

Wave extension : \_flepl

File:

[FlexCyl\\_PolyLen.ipf](#)

Requires:

[GaussUtils.ipf](#)

[PlotUtils.ipf](#)

[FlexibleCylinder.ipf](#)

### AUTHOR/MODIFICATION

Wei-Ren Chen 1 JUL 2006

### APPROVED FOR DISTRIBUTION

Steve Kline 15 JUL 2006

### DESCRIPTION

Calculates the form factor for a flexible cylinder with a circular cross section and a uniform scattering length density. Polydispersity of the overall contour length is included, using a Schulz distribution. The non-negligible diameter of the cylinder is included by accounting for excluded volume interactions within the walk of a single cylinder. Inter-cylinder interactions are NOT included. The form factor is normalized by

the particle volume such that  $P(q) = \text{scale} \cdot \langle f^2 \rangle / \text{Vol} + \text{bkg}$ , where  $\langle \rangle$  is an average over all possible orientations of the flexible cylinder. An instrument resolution smeared version is also provided.

## VARIABLES

Input Variables (default values):

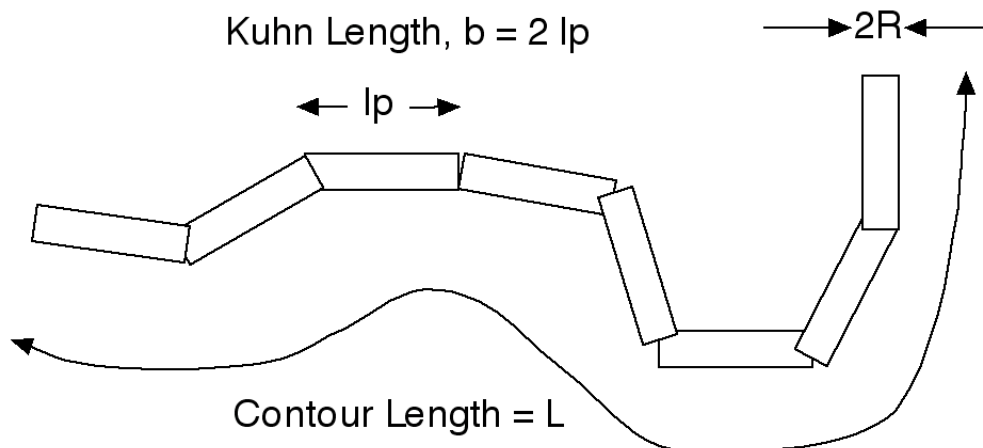
parameters_flepl	coef_flepl
scale	1
Contour Length (A)	1000
polydispersity of Contour Length	0.001
Kuhn Length, b (A)	100
Radius (A)	20
SLD cylinder (A <sup>-2</sup> )	1e-06
SLD solvent (A <sup>-2</sup> )	6.3e-06
bkgd (cm <sup>-1</sup> )	0.0001

## USAGE NOTES

The function calculated is from the reference given below. From that paper, "Method 3 With Excluded Volume" is used. The model is a parametrization of simulations of a discrete representation of the worm-like chain model of Kratky and Porod applied in the pseudocontinuous limit. See equations (13,26-27) in the original reference for the details.

**NOTE:** there are several typos in the original reference that have been corrected by WRC. Details of the corrections are in the reference below.

- Equation (13): the term  $(1-w(QR))$  should swap position with  $w(QR)$
- Equations (23) and (24) are incorrect. WRC has entered these into Mathematica and solved analytically. The results were converted to code.
- Equation (27) should be  $q_0 = \max(a_3/\sqrt{R_g^2}, 3)$  instead of  $\max(a_3*b/\sqrt{R_g^2}, 3)$
- The scattering function is negative for a range of parameter values and q-values that are experimentally accessible. A correction function has been added to give the proper behavior.



The chain of contour length,  $L$ , (the total length) can be described a chain of some number of locally stiff segments of length  $l_p$ . The persistence length,  $l_p$ , is the length along the cylinder over which the flexible cylinder can be considered a rigid rod. the Kuhn length ( $b$ ) used in the model is also used to describe the stiffness of a chain, and is simply  $b = 2 \cdot l_p$ .

Polydispersity is included by integrating the form factor over a Schulz distribution of cylinder contour length. The integration has been normalized by the first moment of the length distribution. This insures that the invariant is constant when the polydispersity is varied and all other structural parameters are held fixed.

The returned value is in units of  $[\text{cm}^{-1}]$ , on absolute scale.

Scattering contrast ( $\Delta\rho$ ) = SLD (chain) - SLD (solvent)

$w[0]$  (scale) and contrast are both multiplicative factors in the model and are perfectly correlated. One or both of these parameters must be held fixed during model fitting.

If the scale factor  $w[0]$  is set equal to the particle volume fraction,  $\phi$ , the returned value is the scattered intensity per unit volume,  $I(q) = \phi \cdot P(q)$ . However, no interparticle interference effects are included in this calculation.

## REFERENCE

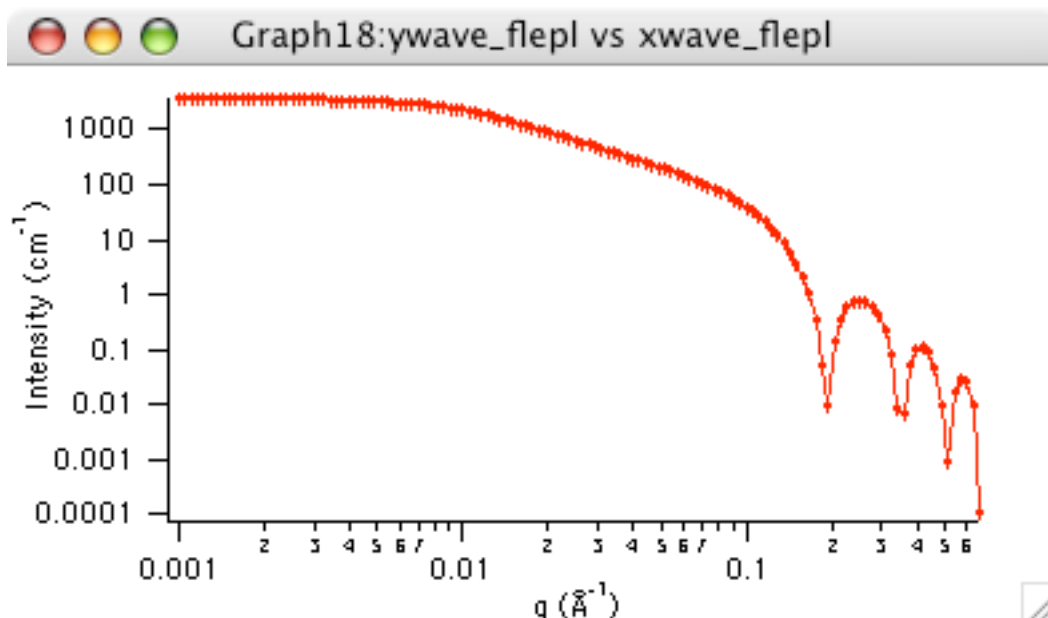
Pedersen, J. S. and P. Schurtenberger (1996). "Scattering functions of semiflexible polymers with and without excluded volume effects." *Macromolecules* 29: 7602-7612.

Corrections are in:

Wei-Ren Chen, Paul D. Butler, and Linda J. Magid, "Incorporating Intermicellar Interactions in the Fitting of SANS Data from Cationic Wormlike Micelles" *Langmuir*, August 2006.

## TEST DATASET

This example dataset is produced by running the Macro `PlotFlexCyl_PolyLength()`, using 128 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.7 \text{ \AA}^{-1}$  and the above default `coef_flepl` values.



### Flexible Cylinder - Polydisperse Radius

#### **MACRO : FUNCTION**

PlotFlexCyl\_PolyRadius() : FlexCylPolyRad(w,y,x)

Wave extension : \_fcpr

File:

[FlexCyl\\_PolyRadius.ipf](#)

Requires:

GaussUtils.ipf

PlotUtils.ipf

[FlexibleCylinder.ipf](#)

#### **AUTHOR/MODIFICATION**

Wei-Ren Chen 1 JUL 2006

#### **APPROVED FOR DISTRIBUTION**

Steve Kline 15 JUL 2006

#### **DESCRIPTION**

Calculates the form factor for a flexible cylinder with a circular cross section and a uniform scattering length density. Polydispersity of the cross-section is included, using a Schulz distribution. The non-negligible diameter of the cylinder is included by accounting for excluded volume interactions within the walk of a single cylinder. Inter-cylinder interactions are NOT included. The form factor is normalized by the particle volume such that  $P(q) = \text{scale} \cdot \langle f^2 \rangle / \text{Vol} + \text{bkg}$ , where  $\langle \rangle$  is an average over all possible orientations of the flexible cylinder. An instrument resolution smeared version is also provided.

#### **VARIABLES**

Input Variables (default values):

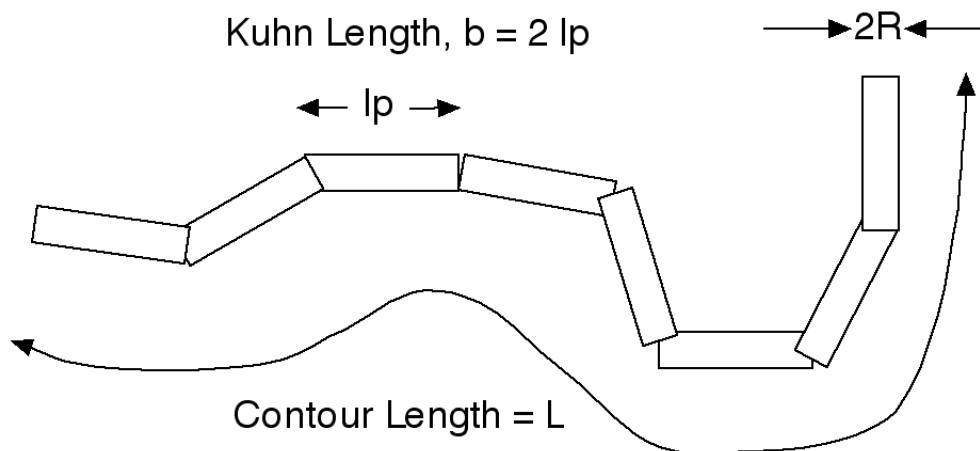
parameters_fcpr	coef_fcpr
scale	1
Contour Length (A)	1000
Kuhn Length, b (A)	100
Radius (A)	20
polydispersity of radius	0.2
SLD cylinder (A <sup>-2</sup> )	1e-06
SLD solvent (A <sup>-2</sup> )	6.3e-06
bkgd (cm <sup>-1</sup> )	0.0001

## USAGE NOTES

The function calculated is from the reference given below. From that paper, "Method 3 With Excluded Volume" is used. The model is a parametrization of simulations of a discrete representation of the worm-like chain model of Kratky and Porod applied in the pseudocontinuous limit. See equations (13,26-27) in the original reference for the details.

**NOTE:** there are several typos in the original reference that have been corrected by WRC. Details of the corrections are in the reference below.

- Equation (13): the term  $(1-w(QR))$  should swap position with  $w(QR)$
- Equations (23) and (24) are incorrect. WRC has entered these into Mathematica and solved analytically. The results were converted to code.
- Equation (27) should be  $q_0 = \max(a_3/\sqrt{R_g^2}, 3)$  instead of  $\max(a_3*b/\sqrt{R_g^2}, 3)$
- The scattering function is negative for a range of parameter values and q-values that are experimentally accessible. A correction function has been added to give the proper behavior.



The chain of contour length,  $L$ , (the total length) can be described a chain of some number of locally stiff segments of length  $l_p$ . The persistence length,  $l_p$ , is the length along the cylinder over which the flexible cylinder can be considered a rigid rod. the Kuhn length ( $b$ ) used in the model is also used to describe the stiffness of a chain, and is simply  $b = 2 * l_p$ .

Polydispersity is included by integrating the form factor over a Schulz distribution of cylinder radius. The integration has been normalized by the second moment of the radius distribution. This insures that the invariant is constant when the polydispersity is varied and all other structural parameters are held fixed.

The returned value is in units of  $[\text{cm}^{-1}]$ , on absolute scale.

Scattering contrast ( $\Delta\rho$ ) = SLD (chain) - SLD (solvent)

$w[0]$  (scale) and contrast are both multiplicative factors in the model and are perfectly correlated. One or both of these parameters must be held fixed during model fitting.

If the scale factor  $w[0]$  is set equal to the particle volume fraction,  $\phi$ , the returned value is the scattered intensity per unit volume,  $I(q) = \phi * P(q)$ . However, no interparticle interference effects are included in this calculation.

## REFERENCE

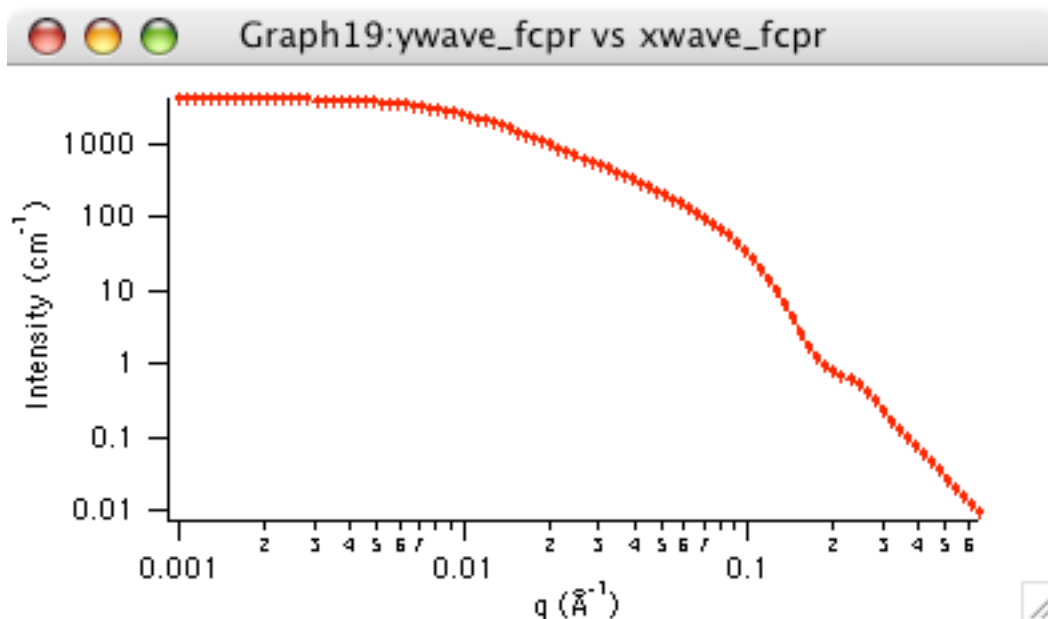
Pedersen, J. S. and P. Schurtenberger (1996). "Scattering functions of semiflexible polymers with and without excluded volume effects." *Macromolecules* 29: 7602-7612.

Corrections are in:

Wei-Ren Chen, Paul D. Butler, and Linda J. Magid, "Incorporating Intermicellar Interactions in the Fitting of SANS Data from Cationic Wormlike Micelles" *Langmuir*, August 2006.

## TEST DATASET

This example dataset is produced by running the Macro PlotFlexCyl\_PolyRadius(), using 100 data points,  $q_{\text{min}} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\text{max}} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_fcpr values.





## Ellipsoid of Revolution

### MACRO : FUNCTION

PlotEllipsoidForm() : EllipsoidForm(w,y,x)

Wave extension: \_eor

File:

UniformEllipsoid.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

### AUTHOR/MODIFICATION

Steve Kline 20 JAN 1999

### APPROVED FOR DISTRIBUTION

Sungmin Choi 02 FEB 1999

### DESCRIPTION

Calculates the form factor for a monodisperse ellipsoid (ellipsoid of revolution) with uniform scattering length density. The form factor is normalized by the particle volume such that  $P(q) = \text{scale} \cdot \langle f^2 \rangle / \text{Vol} + \text{bkg}$ , where  $f$  is the scattering amplitude and the  $\langle \rangle$  denote an average over all possible orientations of the ellipsoid. Resolution smeared version is also provided.

### VARIABLES

Input Variables (default values):

parameters_eor	coef_eor
scale	1
R a (rotation axis) (Å)	20
R b (Å)	400
SLD ellipsoid (Å <sup>-2</sup> )	1e-06
SLD solvent (Å <sup>-2</sup> )	6.3e-06
incoh. bkg (cm <sup>-1</sup> )	0.01

### USAGE NOTES

The function calculated is:

$$P(q) = \frac{\text{scale}}{V_{\text{ell}}} (\rho_{\text{ell}} - \rho_{\text{solv}})^2 \int_0^1 f^2 [q r_b (1 + x^2 (v^2 - 1))^{1/2}] dx + \text{bkg}$$

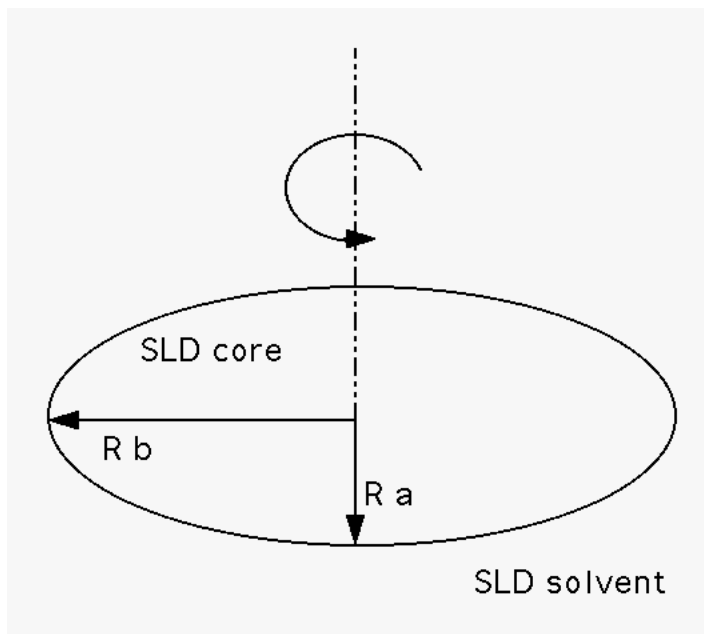
$$f(z) = 3V_{\text{ell}} \frac{(\sin z - z \cos z)}{z^3}$$

$$V_{\text{ell}} = \frac{4\pi}{3} r_a r_b^2 \quad \text{and} \quad v = \frac{r_a}{r_b}$$

The returned value is scaled to units of [cm<sup>-1</sup>], on absolute scale.

The ellipse is rotated about the axis of Ra to define the ellipsoid. If (as shown below) the

radius  $R_b > R_a$ , the object is an oblate ellipsoid (disk-like). If  $R_b < R_a$ , then the object is a prolate ellipsoid (needle-like). If the two radii are equal, then the ellipsoid is a sphere.



If the object is an oblate ellipsoid (disk-like), it displays a limiting power-law slope of  $q^{-2}$  at low  $q$ .

A prolate ellipsoid (needle-like), displays a limiting power-law slope of  $q^{-1}$  at low  $q$ .

$w[0]$  (scale) and contrast are both multiplicative factors in the model and are perfectly correlated. One or both of these parameters must be held fixed during model fitting.

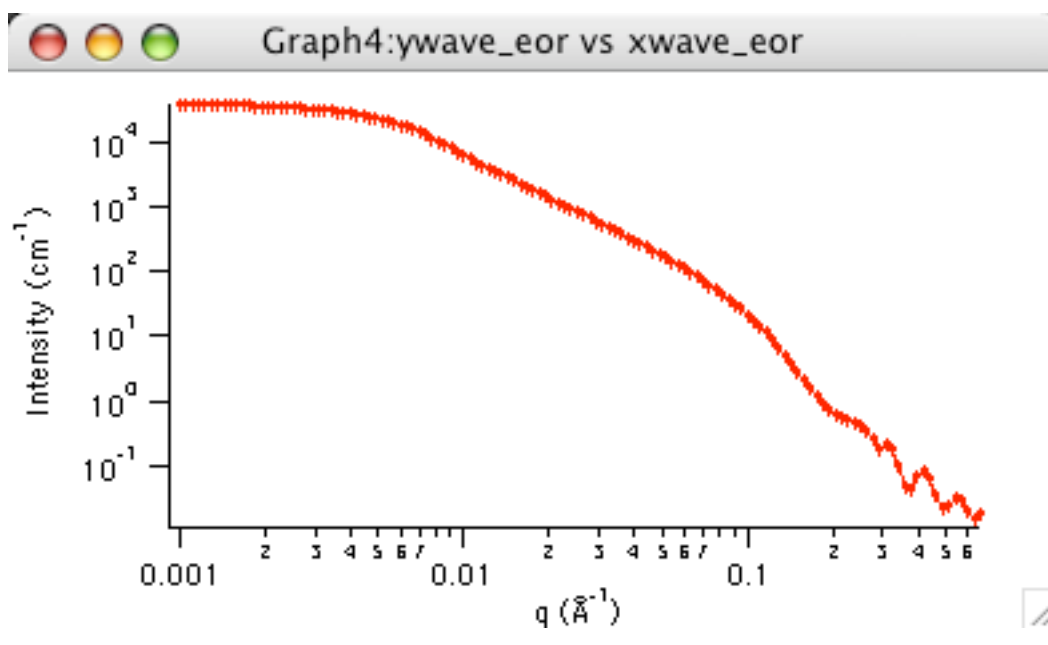
If the scale factor  $w[0]$  is set equal to the particle volume fraction,  $\phi$ , the returned value is the scattered intensity per unit volume,  $I(q) = \phi * P(q)$ . However, no interparticle interference effects are included in this calculation.

## REFERENCE

Feigin, L. A, and D. I. Svergun, "Structure Analysis by Small-Angle X-Ray and Neutron Scattering", Plenum Press, New York, (1987).

## TEST DATASET

This example dataset is produced by running the Macro PlotEllipsoidForm(), using 128 data points,  $q_{min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_eor values.



### Triaxial Ellipsoid

#### **MACRO : FUNCTION**

Plot\_TriaxialEllipsoid() : TriaxialEllipsoid(w,y,x)

Wave extension: \_triax

File:

TriaxialEllipsoid.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

#### **AUTHOR/MODIFICATION**

Steve Kline 5 DEC 2000

#### **APPROVED FOR DISTRIBUTION**

Derek Ho 2 DEC 2003

#### **DESCRIPTION**

Calculates the form factor for a triaxial ellipsoid with uniform scattering length density. The form factor is normalized by the particle volume such that  $P(q) = \text{scale} \cdot \langle f^2 \rangle / \text{Vol} + \text{bkg}$ , where  $\langle \rangle$  is an average over all possible orientations of the ellipsoid. An instrument resolution smeared version is also provided.

#### **VARIABLES**

Input Variables (default values):

parameters_triax	coef_triax
Scale Factor	1
Semi-axis A [smallest](Å)	35
Semi-axis B (Å)	100
Semi-axis C [largest](Å)	400
SLD ellipsoid (Å <sup>-2</sup> )	1e-06
SLD solvent (Å <sup>-2</sup> )	6.3e-06
Incoherent Bgd (cm <sup>-1</sup> )	0

### USAGE NOTES

The function calculated is for an ellipsoid where all three semi-axes are of different lengths. For the results of the calculation to be valid, the axes MUST be defined as:

$$a \leq b \leq c$$

then:

$$P(q) = \frac{scale}{V_{el}} \int_0^1 \int_0^1 \phi^2 \{ q [a^2 \cos^2(\pi x/2) + b \sin^2(\pi x/2)(1 - y^2) + c^2 y^2]^{1/2} \} dx dy$$

Where the function  $\phi(x)$  is defined as:

$$\phi^2(x) = 9 \left( \frac{\sin x - x \cos x}{x^3} \right)^2$$

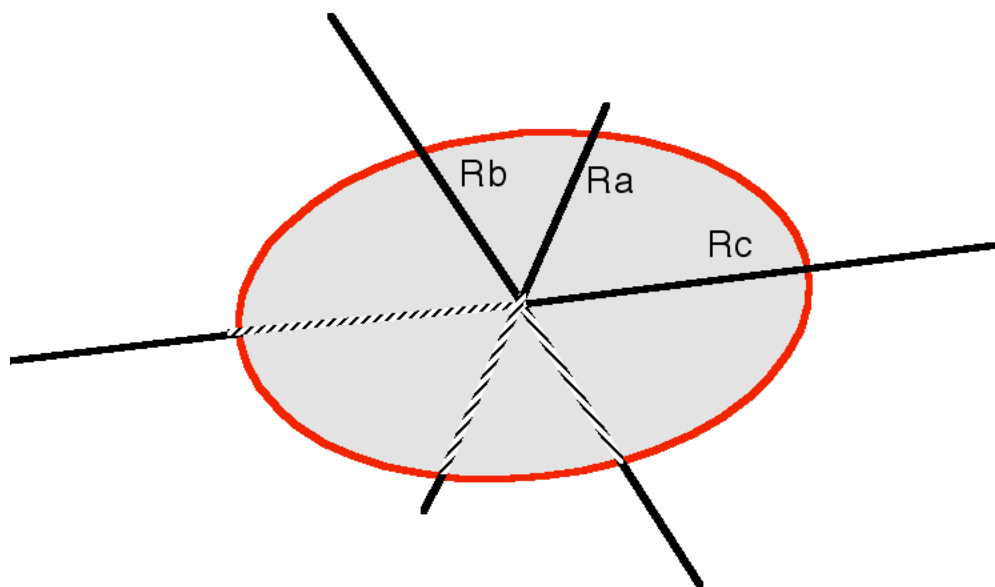
The volume of the ellipsoid is:

$$V_{el} = \frac{4\pi}{3} a b c$$

and its radius of gyration is:

$$R_g^2 = \frac{a^2 + b^2 + c^2}{5}$$

The returned value is in units of [cm<sup>-1</sup>], on absolute scale.



#### NOTES:

Constraints must be applied during fitting to ensure that the inequality  $a < b < c$  is not violated. The calculation will not report an error, but the results will not be correct.

Scattering contrast ( $\Delta\rho$ ) = SLD (ellipsoid) - SLD (solvent)

$w[0]$  (scale) and contrast are both multiplicative factors in the model and are perfectly correlated. One or both of these parameters must be held fixed during model fitting.

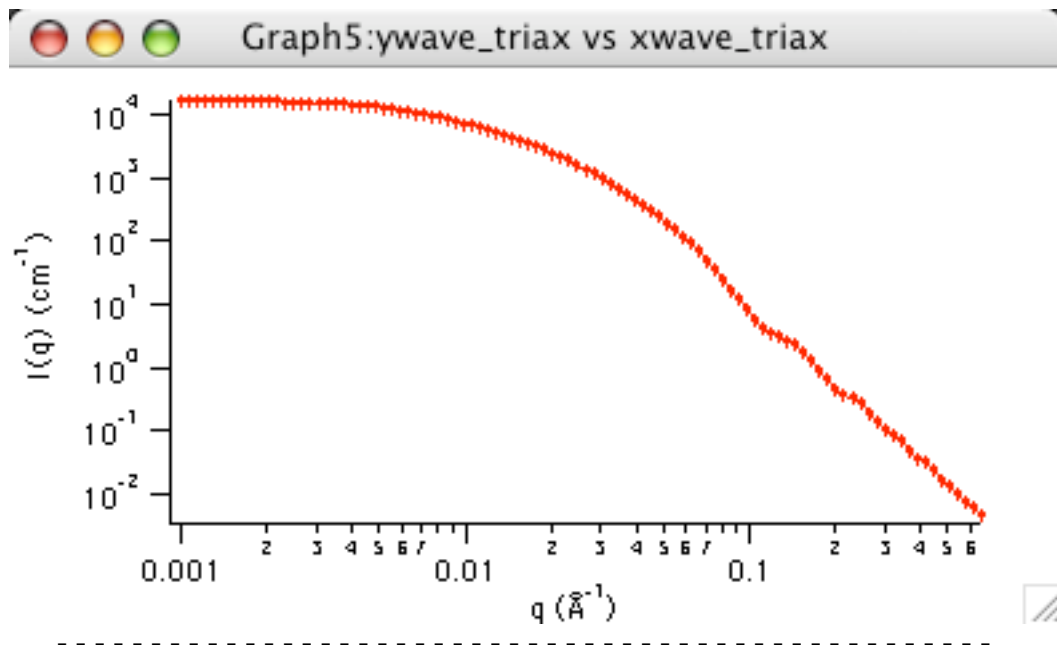
If the scale factor  $w[0]$  is set equal to the particle volume fraction,  $\phi$ , the returned value is the scattered intensity per unit volume,  $I(q) = \phi * P(q)$ . However, no interparticle interference effects are included in this calculation.

#### REFERENCE

L. A. Feigin and D. I. Svergun "Structure Analysis by Small-Angle X-Ray and Neutron Scattering", Plenum, New York, 1987.

#### TEST DATASET

This example dataset is produced by running the Macro Plot\_TriaxialEllipsoid(), using 100 data points,  $q_{min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_triax values.



### Oblate Core-Shell Ellipsoid

#### **MACRO : FUNCTION**

PlotOblateForm() : OblateForm(w,y,x)

Wave extension: \_oef

File:

OblateCoreShell.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

#### **AUTHOR/MODIFICATION**

Steve Kline 06 NOV 1998

#### **APPROVED FOR DISTRIBUTION**

Sungmin Choi 02 FEB 1999

#### **DESCRIPTION**

Calculates the form factor for an oblate ellipsoid particle with a core/shell structure. The form factor is averaged over all possible orientations of the ellipsoid such that  $P(q) = \text{scale} \cdot \langle f^2 \rangle / \text{Vol} + \text{bkg}$ , where  $f$  is the single particle scattering amplitude and the  $\langle \rangle$  represent the orientational average. Resolution smeared version is also provided.

#### **VARIABLES**

Input Variables (default values):

parameters_oef	coef_oef
scale	1
major core (A)	200
minor core (A)	20
major shell (A)	250
minor shell (A)	30
SLD core (A-2)	1e-06
SLD shell (A-2)	2e-06
SLD solvent (A^-2)	6.3e-06
bkg (cm-1)	0.001

### USAGE NOTES

The function calculated is:

$$P(q) = \frac{scale}{V_{shell}} \int_0^1 |F(q, r_i, \alpha)|^2 d\alpha + bkg$$

$$F(q, r_i, \alpha) = 3(\rho_{core} - \rho_{shell}) V_{core} j_1(u_{core}) / u_{core} + 3(\rho_{shell} - \rho_{solv}) V_{shell} j_1(u_{shell}) / u_{shell}$$

where

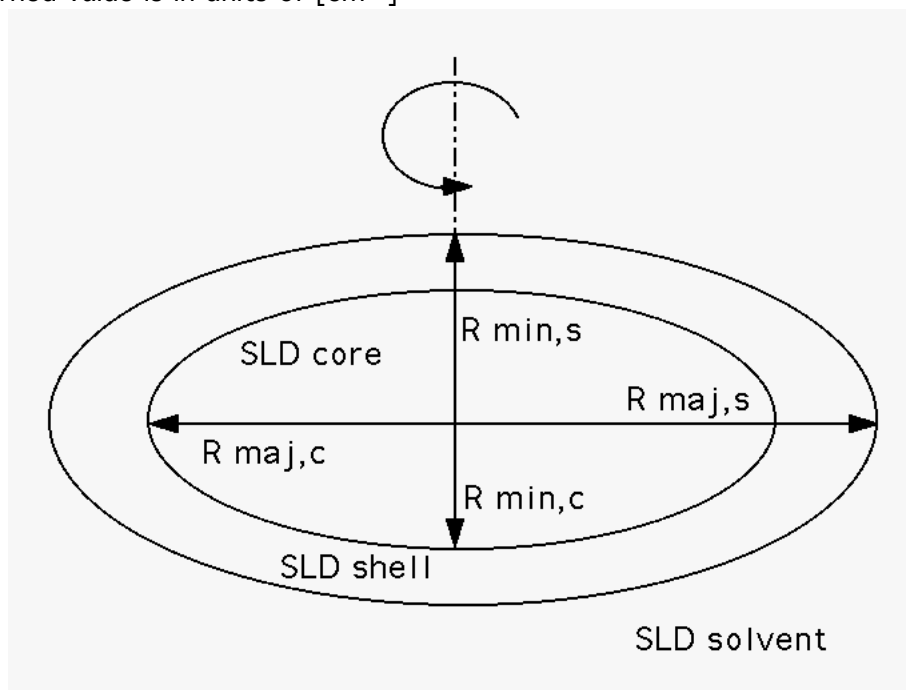
$$V_{core} = (4\pi/3) r_{min,c}^2 r_{maj,c}^2 \quad V_{shell} = (4\pi/3) r_{min,s}^2 r_{maj,s}^2$$

$$u_{core} = q [r_{maj,c}^2 (1 - \alpha^2) + r_{min,c}^2 \alpha^2]^{1/2} \quad u_{shell} = q [r_{maj,s}^2 (1 - \alpha^2) + r_{min,s}^2 \alpha^2]^{1/2}$$

and

$$j_1(x) = (\sin x - x \cos x) / x^2$$

The returned value is in units of [cm<sup>-1</sup>]



Scattering contrast = SLD (core) - SLD (shell) or (shell -solvent) as marked

w[0] (scale), and contrasts are both multiplicative factors in the model and are perfectly correlated. No more than one of these parameters can be free during model fitting.

If the scale factor w[0] is set equal to the particle volume fraction,  $\phi$ , the returned value is the scattered intensity per unit volume,  $I(q) = \phi * P(q)$ . However, no interparticle interference effects are included in this calculation.

It is the users' responsibility to ensure that shell radii are larger than core radii, and that major radii are larger than minor radii.

76-point Gaussian quadrature is used to perform the orientational averaging, so the calculation may be slow on older machines.

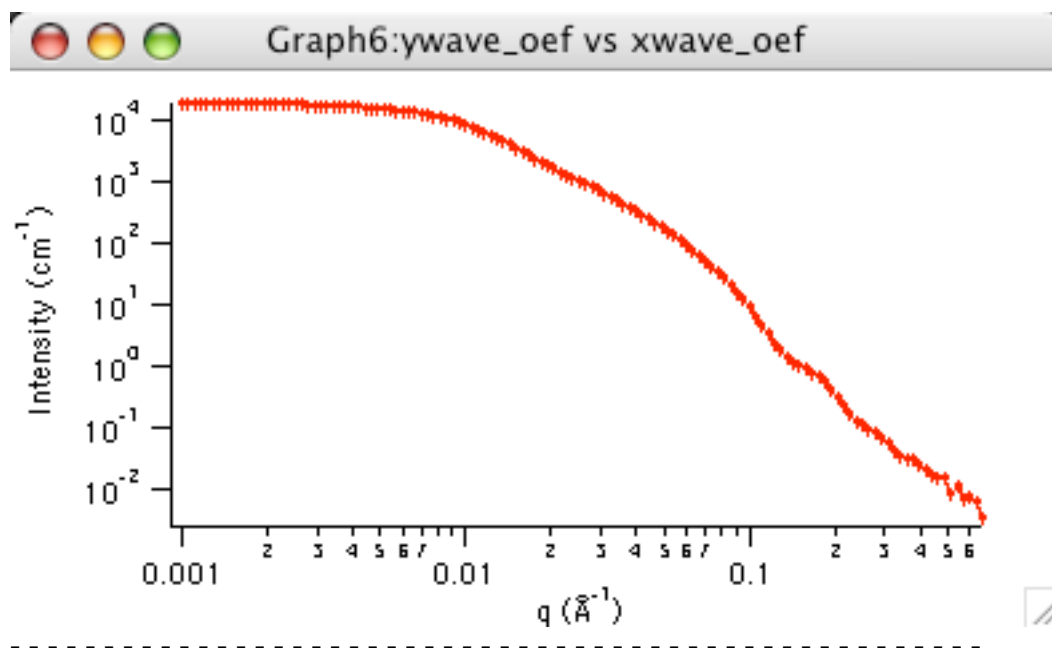
## REFERENCE

Kotlarchyk, M.; Chen, S.-H. *J. Chem. Phys.*, **1983**, 79, 2461.

Berr, S. *J. Phys. Chem.*, **1987**, 91, 4760.

## TEST DATASET

This example dataset is produced by running the Macro PlotOblateForm(), using 128 data points,  $q_{min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_oef values.



## Prolate Core-Shell Ellipsoid

### MACRO : FUNCTION

PlotProlateForm() : ProlateForm(w,y,x)

Wave extension: \_pef

File:

ProlateCoreShell.ipf

Requires:

GaussUtils.ipf



**AUTHOR/MODIFICATION**

Steve Kline 06 NOV 1998

**APPROVED FOR DISTRIBUTION**

Sungmin Choi 02 FEB 1999

**DESCRIPTION**

Calculates the form factor for a monodisperse prolate ellipsoid particle with a core/shell structure. The form factor is averaged over all possible orientations of the ellipsoid. The form factor is normalized by the total particle volume such that  $P(q) = \text{scale} \cdot \langle f^2 \rangle / \text{Vol} + \text{bkg}$ , where  $f$  is the single particle scattering amplitude and the  $\langle \rangle$  represent the orientational average. Resolution smeared version is also provided.

**VARIABLES**

Input Variables (default values):

parameters_pef	coef_pef
scale	1
major core radius (A)	100
minor core radius (A)	50
major shell radius (A)	110
minor shell radius (A)	60
SLD core (A-2)	1e-06
SLD shell (A-2)	2e-06
SLD solvent (A-2)	6.3e-06
bkg (cm-1)	0.001

**USAGE NOTES**The function calculated is  $P(q)$ :

$$P(q) = \frac{\text{scale}}{V} \int_0^1 |F(q, r_{\min}, r_{\text{maj}}, \alpha)|^2 d\alpha + \text{bkg}$$

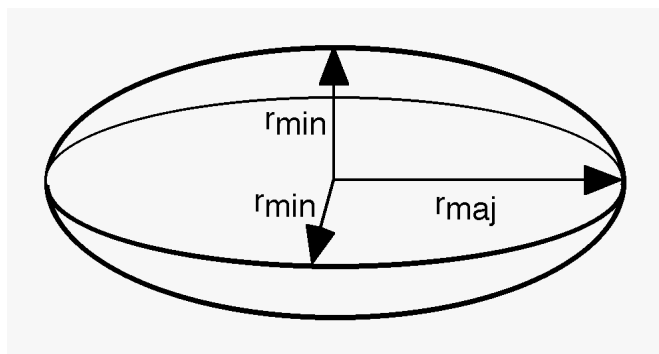
$$F(q, r_{\min}, r_{\text{maj}}, \alpha) = V(r_{\min}, r_{\text{maj}})(\Delta\rho)3j_1(u)/u$$

$$u = q \left[ r_{\text{maj}}^2 \alpha^2 + r_{\min}^2 (1 - \alpha^2) \right]^{1/2}$$

$$V(r_{\min}, r_{\text{maj}}) = (4\pi/3)r_{\text{maj}}r_{\min}^2$$

$$j_1(x) = (\sin x - x \cos x) / x^2$$

The returned value is in units of  $[\text{cm}^{-1}]$



Scattering contrast = SLD (core) - SLD (shell) or SLD (shell -solvent) as marked

$w[0]$  (scale), and contrasts are both multiplicative factors in the model and are perfectly correlated. No more than one of these parameters can be free during model fitting.

If the scale factor  $w[0]$  is set equal to the particle volume fraction,  $\phi$ , the returned value is the scattered intensity per unit volume,  $I(q) = \phi * P(q)$ . However, no interparticle interference effects are included in this calculation.

It is the users' responsibility to ensure that shell radii are larger than core radii, and that major radii are larger than minor radii.

76-point Gaussian quadrature is used to perform the orientational averaging, and may be slow on older machines.

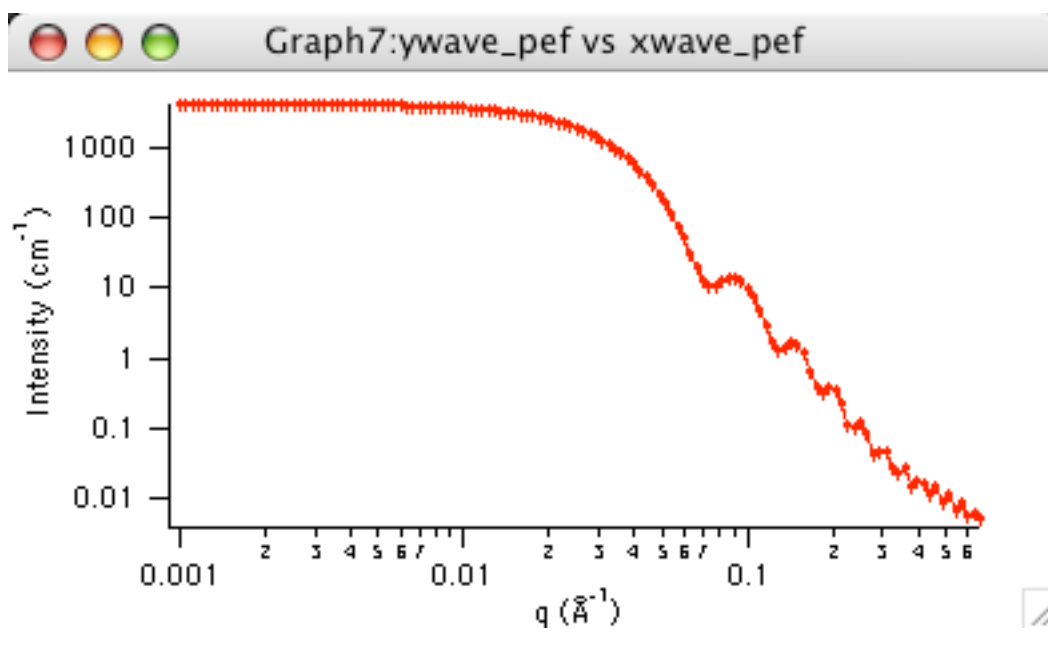
## REFERENCE

Kotlarchyk, M.; Chen, S.-H. *J. Chem. Phys.*, **1983**, 79, 2461.

Berr, S. *J. Phys. Chem.*, **1987**, 91, 4760.

## TEST DATASET

This example dataset is produced by running the Macro PlotProlateForm(), using 128 data points,  $q_{min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_pef values.



## **Parallelepiped**

### **MACRO : FUNCTION**

Plot\_Parallelepiped() : Parallelepiped(w,y,x)

Wave extension: \_Parallelepiped

File:

Parallelepiped.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

### **AUTHOR/MODIFICATION**

Steve Kline 5 DEC 2000

### **APPROVED FOR DISTRIBUTION**

Derek Ho 2 DEC 2003

### **DESCRIPTION**

Calculates the form factor for a rectangular solid with uniform scattering length density. The form factor is normalized by the particle volume such that  $P(q) = \text{scale} \cdot \langle f^2 \rangle / \text{Vol} + \text{bkg}$ , where  $\langle \rangle$  is an average over all possible orientations of the rectangular solid. An instrument resolution smeared version is also provided.

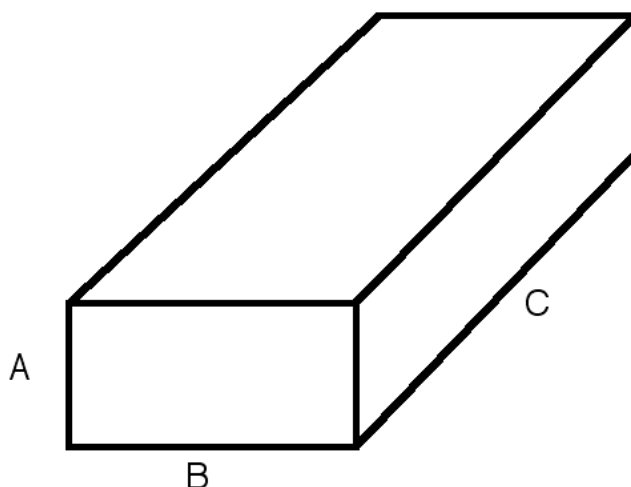
### **VARIABLES**

Input Variables (default values):

parameters_Parallelepiped	coef_Parallelepiped
Scale Factor	1
Shortest Edge A (Å)	35
B (Å)	75
Longest Edge C (Å)	400
SLD particle (Å <sup>-2</sup> )	1e-06
SLD solvent (Å <sup>-2</sup> )	6.3e-06
Incoherent Bgd (cm <sup>-1</sup> )	0

## USAGE NOTES

The function calculated is the form factor of the rectangular solid below:



The volume of the solid is  $V = ABC$ . For the calculation of the form factor to be valid, the sides of the solid MUST be chosen such that  $A < B < C$ . If this inequality is not satisfied, the model will not report an error, and the calculation will not be correct.

Note that the equations that follow are written in terms of reduced lengths, normalized to the middle length, B. By these definitions,  $a < 1$ , and  $c > 1$

$$a = \frac{A}{B} \quad ; \quad b = \frac{B}{B} \equiv 1 \quad ; \quad c = \frac{C}{B}$$

The form factor is then calculated as (a numerical double integral):

$$P(q) = \frac{scale}{V_p} \int_0^1 \phi_Q(\mu \sqrt{1-\sigma^2}, a) [S(\mu c \sigma / 2)]^2 d\sigma$$

$$\phi_Q(\mu, a) = \int_0^1 \left\{ S\left[\frac{\mu}{2} \cos\left(\frac{\pi}{2} u\right)\right] \cdot S\left[\frac{\mu a}{2} \sin\left(\frac{\pi}{2} u\right)\right] \right\}^2 du$$

Where the function  $S(x)$  is defined as:

$$S(x) = \frac{\sin x}{x}$$

and

$$\mu = qB$$

The radius of gyration of a rectangular solid is:

$$R_g^2 = \frac{A^2 + B^2 + C^2}{12}$$

#### FITTING NOTES:

Scattering contrast ( $\Delta\rho$ ) = SLD (parallelepiped) - SLD (solvent)

$w[0]$  (scale) and contrast are both multiplicative factors in the model and are perfectly correlated. One or both of these parameters must be held fixed during model fitting.

If the scale factor  $w[0]$  is set equal to the particle volume fraction,  $\phi$ , the returned value is the scattered intensity per unit volume,  $I(q) = \phi * P(q)$ . However, no interparticle interference effects are included in this calculation.

Constraints must be applied during fitting to ensure that the inequality  $A < B < C$  is not violated. The calculation will not report an error, but the results will not be correct.

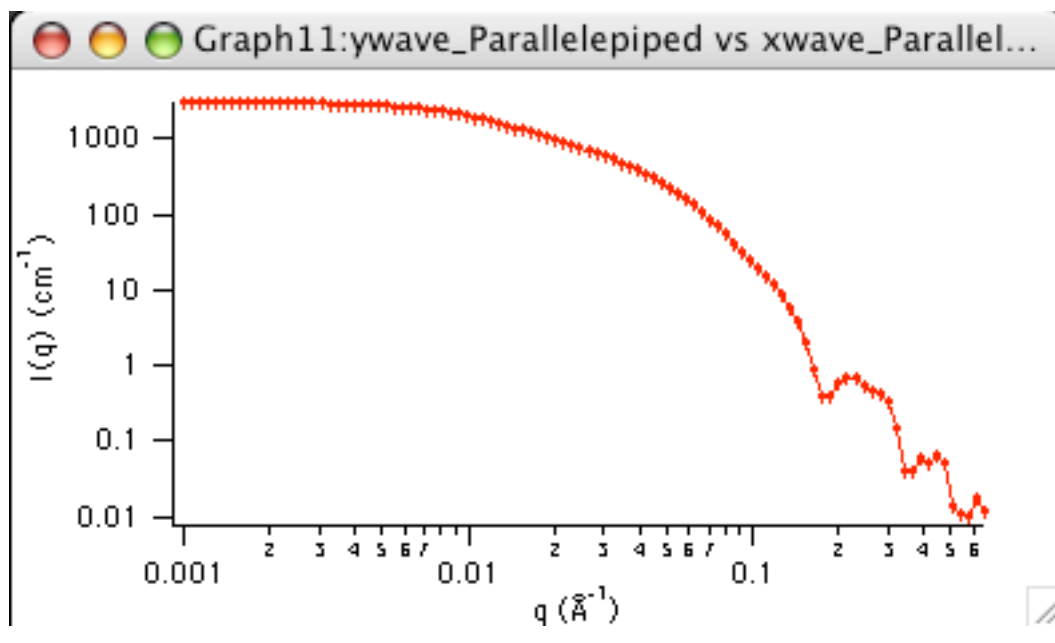
The returned value is in units of  $[\text{cm}^{-1}]$ , on absolute scale.

#### REFERENCE

see: Mittelbach and Porod, Acta Physica Austriaca 14 (1961) 185-211.  
Equations (1), (13-14). (yes, it's in German)

#### TEST DATASET

This example dataset is produced by running the Macro Plot\_Parallelepiped(), using 100 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_Parallelepiped values.



### Dilute Lamellar Form Factor

#### **MACRO : FUNCTION**

Plot\_LamellarFF() : LamellarFF(w,y,x)

Wave extension : \_LamellarFF

File:

LamellarFF.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

#### **AUTHOR/MODIFICATION**

Steve Kline 16 JUL 2003

#### **APPROVED FOR DISTRIBUTION**

Lionel Porcar 6 NOV 2003

#### **DESCRIPTION**

Calculates the form factor from a lyotropic lamellar phase. The intensity calculated is for lamellae of uniform scattering length density that are randomly distributed in solution (a powder average). The thickness of the lamellae is polydisperse. No inter-lamellar structure factor is calculated. Other models are available where  $S(q)$  is calculated. A resolution smeared form factor is provided.

#### **VARIABLES**

Input Variables (default values):

parameters_LamellarFF	coef_LamellarFF
Scale	1
Bilayer Thick (delta) (Å)	50
polydisp of thickness	0.15
SLD bilayer (Å <sup>-2</sup> )	1e-06
SLD solvent (Å <sup>-2</sup> )	6.3e-06
Incoherent Bgd (cm <sup>-1</sup> )	0

## USAGE NOTES

The returned value is  $\text{scale} \cdot I(q) + \text{background}$ , and is in units of  $[\text{cm}^{-1}]$

$$I(q) = \frac{2\pi P(q)}{\delta q^2}$$

where the form factor is given by:

$$P(q) = \frac{2\Delta\rho^2}{q^2} \left[ 1 - \cos(q\delta) e^{-q^2\sigma^2/2} \right]$$

The parameters are:

$\delta$  = bilayer thickness

$\sigma$  = variation in bilayer thickness =  $\delta \cdot \text{polydispersity}$

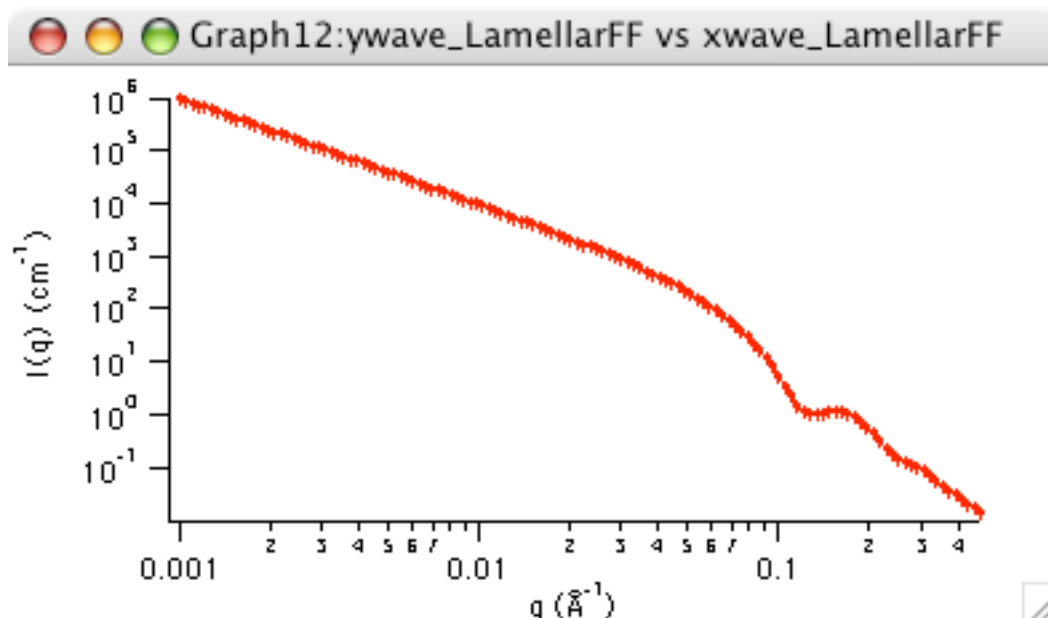
The meaning of the multiplicative scale factor is not well-defined, but should be on the order of the volume fraction of solution occupied by the lamellar crystallites. Please see the original references for clarification.

## REFERENCE

Nallet, Laversanne, and Roux, *J. Phys. II France*, **3**, (1993) 487-502.  
also in *J. Phys. Chem. B*, **105**, (2001) 11081-11088.

## TEST DATASET

This example dataset is produced by running the Macro Plot\_LamellarFF(), using 128 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.5 \text{ \AA}^{-1}$  and the above default coef\_Lamellar values.



#### Dilute Lamellar (head+tail) Form Factor

##### **MACRO : FUNCTION**

Plot\_LamellarFF\_HG() : LamellarFF\_HG(w,y,x)

Wave extension : \_LamellarFF\_HG

File:

LamellarFF\_HG.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

##### **AUTHOR/MODIFICATION**

Steve Kline 16 JUL 2003

##### **APPROVED FOR DISTRIBUTION**

Lionel Porcar 6 NOV 2003

##### **DESCRIPTION**

Calculates the form factor from a lyotropic lamellar phase. The intensity calculated is for lamellae of two-layer scattering length density that are randomly distributed in solution (a powder average). The scattering length density of the tail region, headgroup region, and solvent are taken to be different. No inter-lamellar structure factor is calculated. Other models are available where  $S(q)$  is calculated. A resolution smeared form factor is provided.

##### **VARIABLES**

Input Variables (default values):



Point	parameters_LamellarFF_HG	coef_LamellarFF_HG
0	Scale	1
1	Tail length (Å)	15
2	Headgroup thickness (Å)	10
3	SLD Tails (Å <sup>-2</sup> )	4e-07
4	SLD Headgroup (Å <sup>-2</sup> )	3e-06
5	SLD Solvent (Å <sup>-2</sup> )	6e-06
6	Incoherent Bgd (cm <sup>-1</sup> )	0

## USAGE NOTES

The returned value is  $\text{scale} \cdot I(q) + \text{background}$ , and is in units of  $[\text{cm}^{-1}]$

$$I(q) = \frac{2\pi P(q)}{2(\delta_H + \delta_T)q^2}$$

where the form factor is given by:

$$P(q) = \frac{4}{q^2} \left\{ \Delta\rho_H [\sin[q(\delta_H + \delta_T)] - \sin(q\delta_T)] + \Delta\rho_T \sin(q\delta_T) \right\}^2$$

The parameters are:

$\delta_H$  = headgroup thickness

$\delta_T$  = tail length

$\Delta\rho_H$  = SLD (headgroup) - SLD(solvent)

$\Delta\rho_T$  = SLD (tail) - SLD(headgroup)

NOTE: The total bilayer thickness =  $2(\delta_H + \delta_T)$

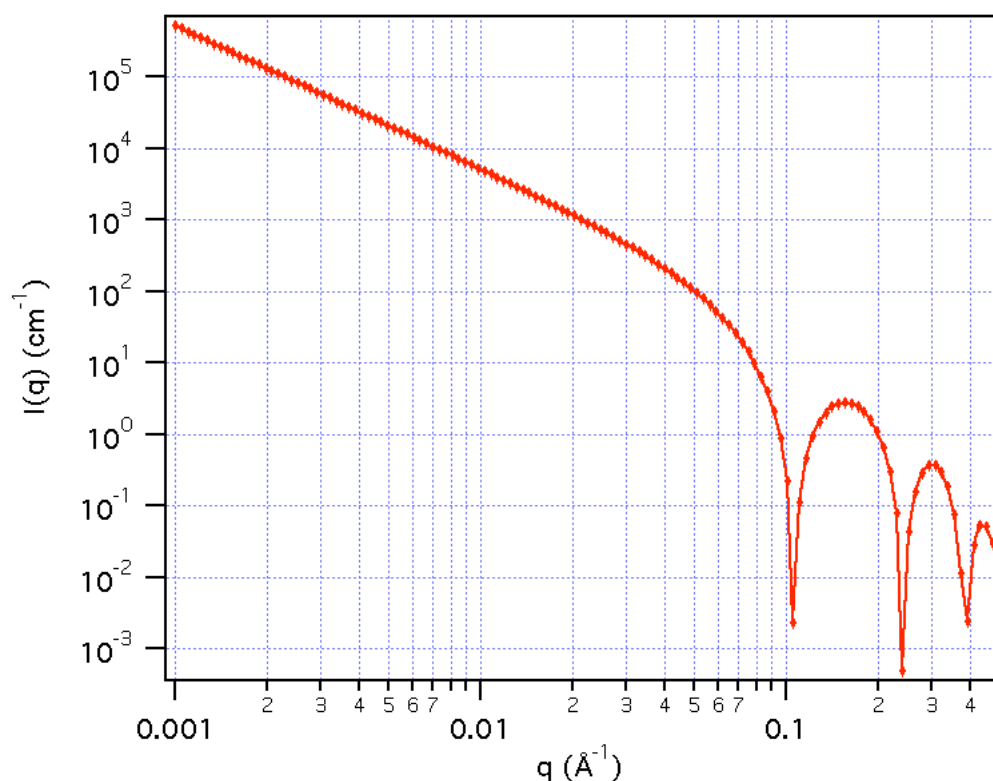
The meaning of the multiplicative scale factor is not well-defined, but should be on the order of the volume fraction of solution occupied by the lamellar crystallites. Please see the original references for clarification.

## REFERENCE

Nallet, Laversanne, and Roux, *J. Phys. II France*, **3**, (1993) 487-502.  
also in *J. Phys. Chem. B*, **105**, (2001) 11081-11088.

## TEST DATASET

This example dataset is produced by running the Macro Plot\_LamellarFF\_HG(), using 128 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.5 \text{ \AA}^{-1}$  and the above default coef\_Lamellar values.



### **Concentrated Lamellar Form Factor**

#### **MACRO : FUNCTION**

Plot\_LamellarPS() : LamellarPS(w,y,x)

Wave extension: \_LamellarPS

File:

LamellarPS.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

#### **AUTHOR/MODIFICATION**

Steve Kline 15 JUL 2003

#### **APPROVED FOR DISTRIBUTION**

Lionel Porcar 6 NOV 2003

#### **DESCRIPTION**

Calculates the scattered intensity from a lyotropic lamellar phase. The intensity (form factor and structure factor) calculated is for lamellae of uniform scattering length density that are randomly distributed in solution (a powder average). The lamellae thickness is polydisperse. The model can also be applied to large, multi-lamellar vesicles (MLV's). A resolution smeared version is provided.

#### **VARIABLES**

Input Variables (default values):

parameters_LamellarPS	coef_LamellarPS
Scale	1
Lamellar spacing, D (Å)	400
Bilayer Thick (delta) (Å)	30
polydisp of Bilayer Thickness	0.15
SLD bilayer (Å <sup>-2</sup> )	1e-06
SLD solvent (Å <sup>-2</sup> )	6.3e-06
# of Lamellar plates	20
Caille parameter	0.1
Incoherent Bgd (cm <sup>-1</sup> )	0

### USAGE NOTES

The returned value is scale\*I(q) + background, and is in units of [cm<sup>-1</sup>]

$$I(q) = \frac{2\pi P(q) S(q)}{dq^2}$$

where the form factor is given by:

$$P(q) = \frac{2\Delta\rho^2}{q^2} \left[ 1 - \cos(q\delta) e^{-q^2\sigma^2/2} \right]$$

and the structure factor for the lamellar stacks is (all terms are part of the summation):

$$S(q) = 1 + 2 \sum_1^{N-1} \left( 1 - \frac{n}{N} \right) \cos \left( \frac{qdn}{1 + 2\Delta q^2 d^2 \alpha(n)} \right) \exp \left( - \frac{2q^2 d^2 \alpha(n) + \Delta q^2 d^2 n^2}{2(1 + 2\Delta q^2 d^2 \alpha(n))} \right) \frac{1}{\sqrt{1 + 2\Delta q^2 d^2 \alpha(n)}}$$

with the Caille parameter:

$$\eta_{cp} = \frac{q_o^2 k_B T}{8\pi \sqrt{KB}}$$

$$\alpha(n) = \frac{\eta_{cp}}{4\pi^2} [\ln(\pi n) + \gamma_E]$$

and Euler's constant:

$$\gamma_E = 0.5772156649$$

The parameters are:

d = repeat spacing

$\delta$  = bilayer thickness

$\Delta q$  = instrumental resolution (==0 if the unsmeared version is plotted)

$\sigma$  = variation in bilayer thickness

K = smectic bending elasticity

B = compression modulus

N = number of lamellar plates (only the integer portion is used)

#### MODEL NOTES:

The meaning of the multiplicative scale factor is not well-defined, but should be on the order of the volume fraction of solution occupied by the lamellar crystallites. Please see the original references for clarification.

The model is only valid for lamellar phases with strong interactions between the membranes.

When the Caille parameter is greater than approximately 0.8 to 1.0, the assumptions of the model are not correct. The calculation will not fail, but the validity of the model calculation is suspect.

The strong scattering predicted at low Q values is a consequence of the powder average of the model ( $1/Q^2$ ) and will tend to overestimate the scattering from a real sample. It is more important that the Bragg peak and any higher order peaks are well fitted.

If it is possible, use the scattering from a dilute lamellar phase and fit with a form factor only model to determine the thickness and polydispersity. Then use those values as fixed inputs to this calculation.

#### NOTES FOR CURVE FITTING:

1) The epsilon wave "epsilon\_LamellarPS" must be used to force a larger derivative step for the # of repeat units, which is an integer. A singular matrix error will always result if you don't follow this. This wave is created and filled with the appropriate values when the "Plot\_LamellarPS" macro is run.

2) The # of repeats should be constrained to approximately  $3 < N < 200$ , otherwise the optimization can pick a VERY large N, and appear to "hang" for long periods of time in the calculation. Do this by specifying a constraint wave (a "New Wave") in the same tab of the Curve Fitting Dialog as where the epsilon wave is specified

3) Only the integer portion of the number of repeats is used. Although a floating point value is reported in the coefficient list, the value is truncated to an integer for the calculation.

#### REFERENCE

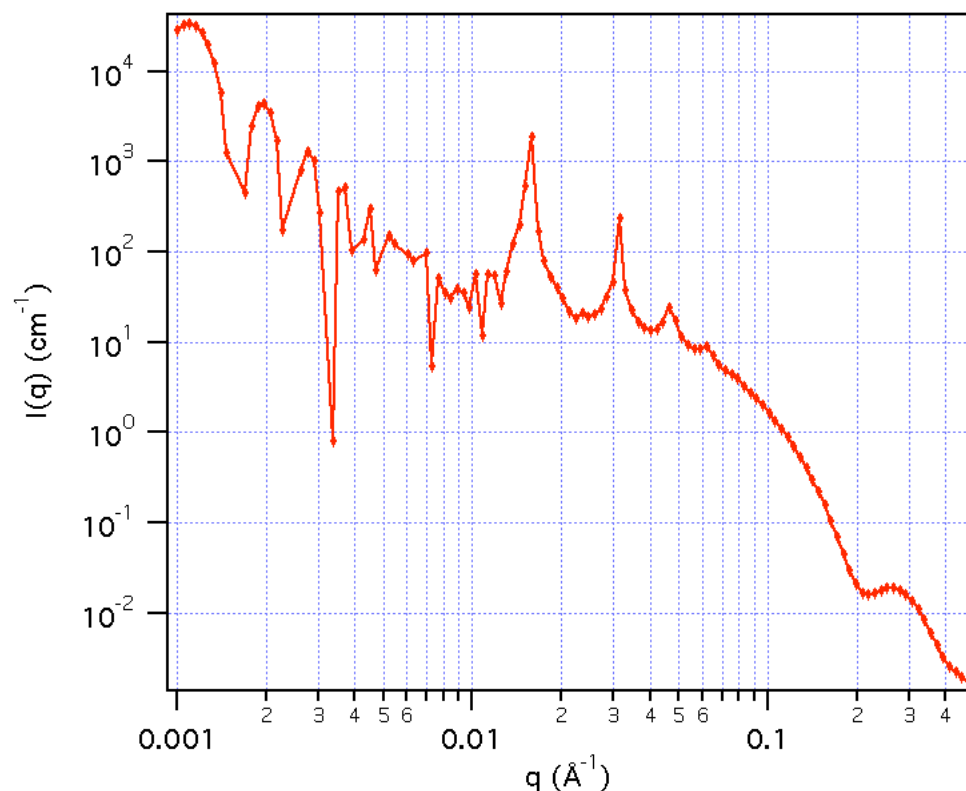
Nallet, Laversanne, and Roux, *J. Phys. II France*, **3**, (1993) 487-502.

also in *J. Phys. Chem. B*, **105**, (2001) 11081-11088.

#### TEST DATASET

This example dataset is produced by running the Macro Plot\_LamellarPS(), using 128

data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.5 \text{ \AA}^{-1}$  and the above default coef\_LamellarPS values. No resolution smearing was used.



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### Concentrated Lamellar (head+tail) Form Factor

#### **MACRO : FUNCTION**

Plot\_LamellarPS\_HG() : LamellarPS\_HG(w,y,x)

Wave extension: \_LamellarPS\_HG

File:

LamellarPS\_HG.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

#### **AUTHOR/MODIFICATION**

Steve Kline 15 JUL 2003

#### **APPROVED FOR DISTRIBUTION**

Lionel Porcar 6 NOV 2003

#### **DESCRIPTION**

Calculates the scattered intensity from a lyotropic lamellar phase. The intensity calculated is for lamellae of two-layer scattering length density that are randomly distributed in solution (a powder average). The scattering length density of the tail

region, headgroup region, and solvent are taken to be different. The model can also be applied to large, multi-lamellar vesicles (MLV's). A resolution smeared version is provided.

## VARIABLES

Input Variables (default values):

Point	parameters_LamellarPS_HG	coef_LamellarPS_HG
0	Scale	1
1	Lamellar spacing, D (Å)	40
2	Tail Thick (delT) (Å)	10
3	HG Thick (delH) (Å)	2
4	SLD of tails (Å <sup>-2</sup> )	4e-07
5	SLD of HG (Å <sup>-2</sup> )	2e-06
6	SLD of solvent (Å <sup>-2</sup> )	6e-06
7	# of Lamellar plates	30
8	Caille parameter	0.001
9	Incoherent Bgd (cm <sup>-1</sup> )	0.001

## USAGE NOTES

The returned value is scale\*I(q) + background, and is in units of [cm<sup>-1</sup>]

$$I(q) = \frac{2\pi P(q) S(q)}{dq^2}$$

where the form factor is given by:

$$P(q) = \frac{4}{q^2} \left\{ \Delta\rho_H [\sin[q(\delta_H + \delta_T)] - \sin(q\delta_T)] + \Delta\rho_T \sin(q\delta_T) \right\}^2$$

and the structure factor for the lamellar stacks is (all terms are part of the summation):

$$S(q) = 1 + 2 \sum_1^{N-1} \left( 1 - \frac{n}{N} \right) \cos \left( \frac{qdn}{1 + 2\Delta q^2 d^2 \alpha(n)} \right) \exp \left( - \frac{2q^2 d^2 \alpha(n) + \Delta q^2 d^2 n^2}{2(1 + 2\Delta q^2 d^2 \alpha(n))} \right) \frac{1}{\sqrt{1 + 2\Delta q^2 d^2 \alpha(n)}}$$

with the Caille parameter:

$$\eta_{cp} = \frac{q_o^2 k_B T}{8\pi \sqrt{KB}}$$

$$\alpha(n) = \frac{\eta_{cp}}{4\pi^2} [\ln(\pi n) + \gamma_E]$$

and Euler's constant:

$$\gamma_E = 0.5772156649$$

The parameters are:

d = repeat spacing

δH = headgroup thickness

δT = tail length

ΔρH = SLD (headgroup) - SLD(solvent)

ΔρT = SLD (tail) - SLD(headgroup)

Δq = instrumental resolution (==0 if unsmeared version is plotted)

K = smectic bending elasticity

B = compression modulus

N = number of lamellar plates (only the integer portion is used)

MODEL NOTES:

The total bilayer thickness = 2(δH + δT)

The meaning of the multiplicative scale factor is not well-defined, but should be on the order of the volume fraction of solution occupied by the lamellar crystallites. Please see the original references for clarification.

The model is only valid for lamellar phases with strong interactions between the membranes.

When the Caille parameter is greater than approximately 0.8 to 1.0, the assumptions of the model are not correct. The calculation will not fail, but the validity of the model calculation is suspect.

The strong scattering predicted at low Q values is a consequence of the powder average of the model (1/Q<sup>2</sup>) and will tend to overestimate the scattering from a real sample. It is more important that the Bragg peak and any higher order peaks are well fitted.

If it is possible, use the scattering from a dilute lamellar phase and fit with a form factor only model to determine the thickness and polydispersity. Then use those values as fixed inputs to this calculation.

The meaning of the multiplicative scale factor is not well-defined, but should be on the order of the volume fraction of solution occupied by the lamellar crystallites. Please see the original references for clarification.

NOTES FOR CURVE FITTING:

1) The epsilon wave "epsilon\_LamellarPS" must be used to force a larger derivative step for the # of repeat units, which is an integer. A singular matrix error will always result if you don't follow this. This wave is created and filled with the

appropriate values when the "Plot\_LamellarPS" macro is run.

2) The # of repeats should be constrained to approximately  $3 < N < 200$ , otherwise the optimization can pick a VERY large N, and appear to "hang" for long periods of time in the calculation. Do this by specifying a constraint wave (a "New Wave") in the same tab of the Curve Fitting Dialog as where the epsilon wave is specified

3) Only the integer portion of the number of repeats is used. Although a floating point value is reported in the coefficient list, the value is truncated to an integer for the calculation.

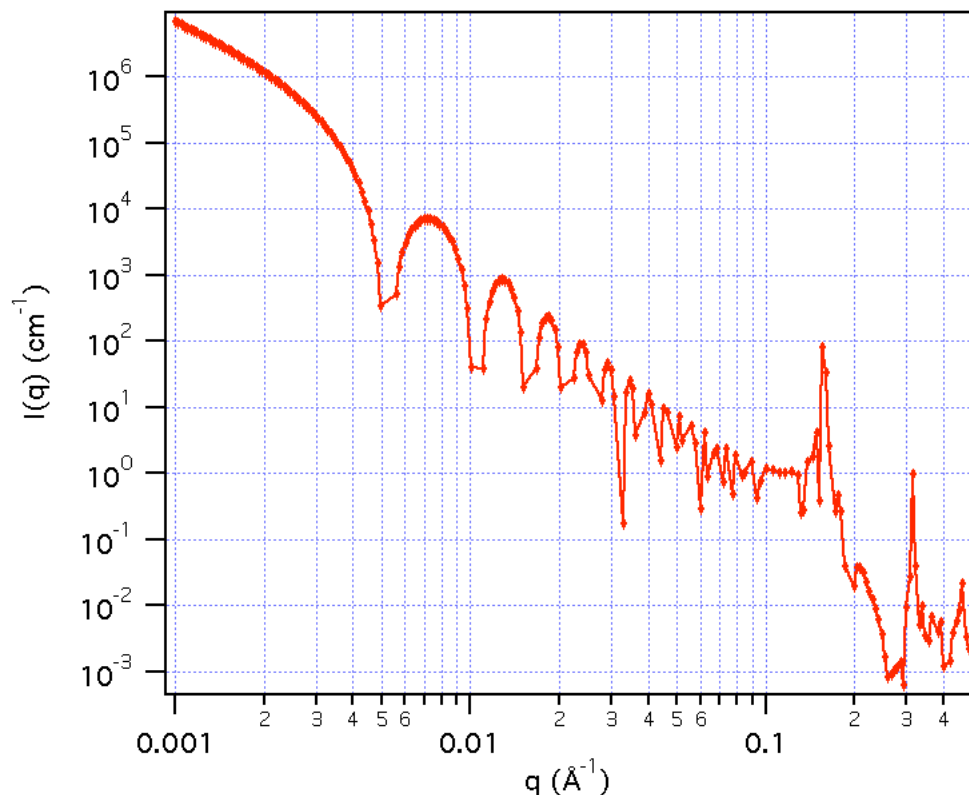
## REFERENCE

Nallet, Laversanne, and Roux, *J. Phys. II France*, **3**, (1993) 487-502.

also in *J. Phys. Chem. B*, **105**, (2001) 11081-11088.

## TEST DATASET

This example dataset is produced by running the Macro Plot\_LamellarPS\_HG(), using 256 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.5 \text{ \AA}^{-1}$  and the above default coef\_LamellarPS\_HG values. No resolution smearing was used.



## Stacked Disks (Tactoids)

### MACRO : FUNCTION

PlotStackedDisks() : StackedDisks(w,y,x)

Wave extension: \_scyl

File:



StackedDiscs.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

## AUTHOR/MODIFICATION

Derek L. Ho 04 JUL 2001

## APPROVED FOR DISTRIBUTION

Steven Kline 10 JUL 2001

## DESCRIPTION

Calculates the total coherent scattered intensity from stacked discs (tactoids) with a core/layer structure. Assuming the next neighbor distance (d-spacing) in a stack of parallel discs obeys a Gaussian distribution, a structure factor  $S(q)$  proposed by Kratky and Porod in 1949 is used in this function. Note that the resolution smearing calculation uses 76 Gauss quadrature points to properly smear the model since the function is HIGHLY oscillatory, especially around the  $q$ -values that correspond to the repeat distance of the layers. This can make the calculations rather slow.

## VARIABLES

Input Variables (default values):

Point	parameters_scyl	coef_scyl
0	scale	0.01
1	Disc Radius (A)	3000
2	Core Thickness (A)	10
3	Layer Thickness (A)	15
4	Core SLD (A <sup>-2</sup> )	4e-06
5	Layer SLD (A <sup>-2</sup> )	-4e-07
6	Solvent SLD (A <sup>-2</sup> )	5e-06
7	# of Stacking	1
8	GSD of d-Spacing	0
9	incoh. bkg (cm <sup>-1</sup> )	0.001

## USAGE NOTES

The function calculated is:

$$I(q) = N \int_0^{\pi/2} \left[ \Delta\rho_i (V_t f_i(q) - V_c f_c(q)) + \Delta\rho_c V_c f_c(q) \right]^2 S(q) \sin\phi d\phi + bkg$$

where  $N$  is the number of discs per unit volume,  $\Delta\rho_i = \rho_i - \rho_{solvent}$  represents the corresponding contrast of species  $i$  with respect to the solvent, and  $\phi$  is the angle between  $q$  and the axis of the disc,

$V_t$  and  $V_c$  are the total volume and the core volume of a single disc, respectively.

$$\langle f_t^2(q) \rangle_\varphi = \int_0^{\pi/2} \left[ \left( \frac{\sin(q(d+h)\cos\varphi)}{q(d+h)\cos\varphi} \right) \left( \frac{2J_1(qR\sin\varphi)}{qR\sin\varphi} \right) \right]^2 \sin\varphi d\varphi$$

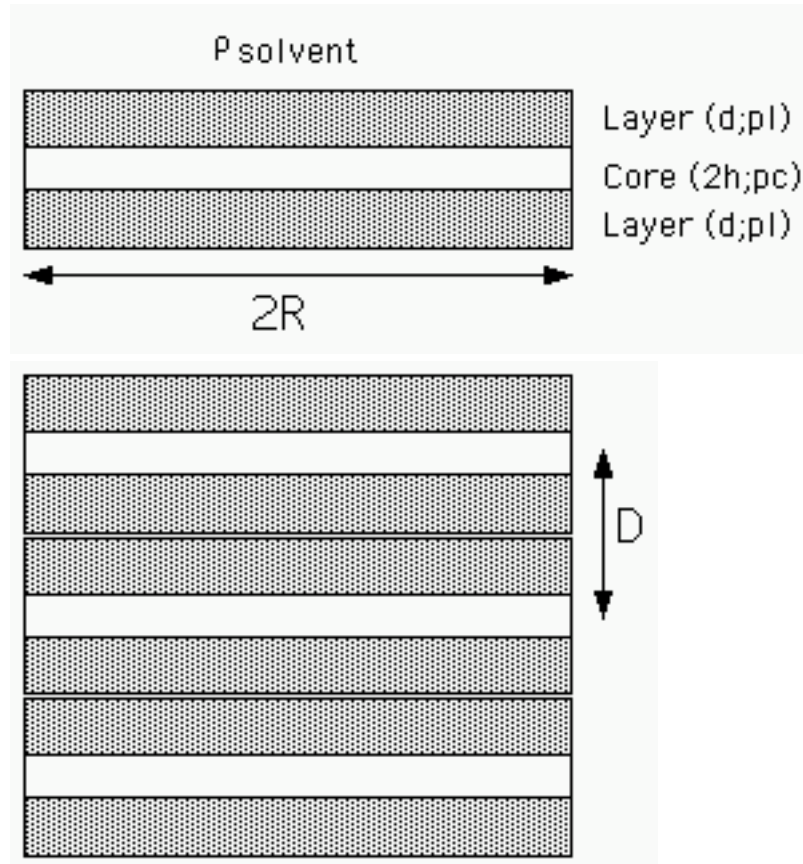
$$\langle f_c^2(q) \rangle_\varphi = \int_0^{\pi/2} \left[ \left( \frac{\sin(qh\cos\varphi)}{qh\cos\varphi} \right) \left( \frac{2J_1(qR\sin\varphi)}{qR\sin\varphi} \right) \right]^2 \sin\varphi d\varphi$$

where d, 2h and R are the thickness of the layer, the core thickness and the radius of the disc, respectively.

$$S(q) = 1 + \frac{2}{n} \sum_{k=1}^n (n-k) \cos(kDq \cos\varphi) \exp[-k(q \cos\varphi)^2 \sigma_D^2 / 2]$$

where n corresponds to the total number of discs stacked, and D and  $\sigma_D$  represent the next neighbor center-to-center distance (d-spacing) and its Gaussian standard deviation (GSD), respectively.

The returned value is scaled to units of  $[\text{cm}^{-1}]$ .



Scattering from fully exfoliated monodisperse discs (the single disc form factor  $P(q)$ ) can be calculated by setting the total number of discs stacked per tactoid equal to 1.

## REFERENCE

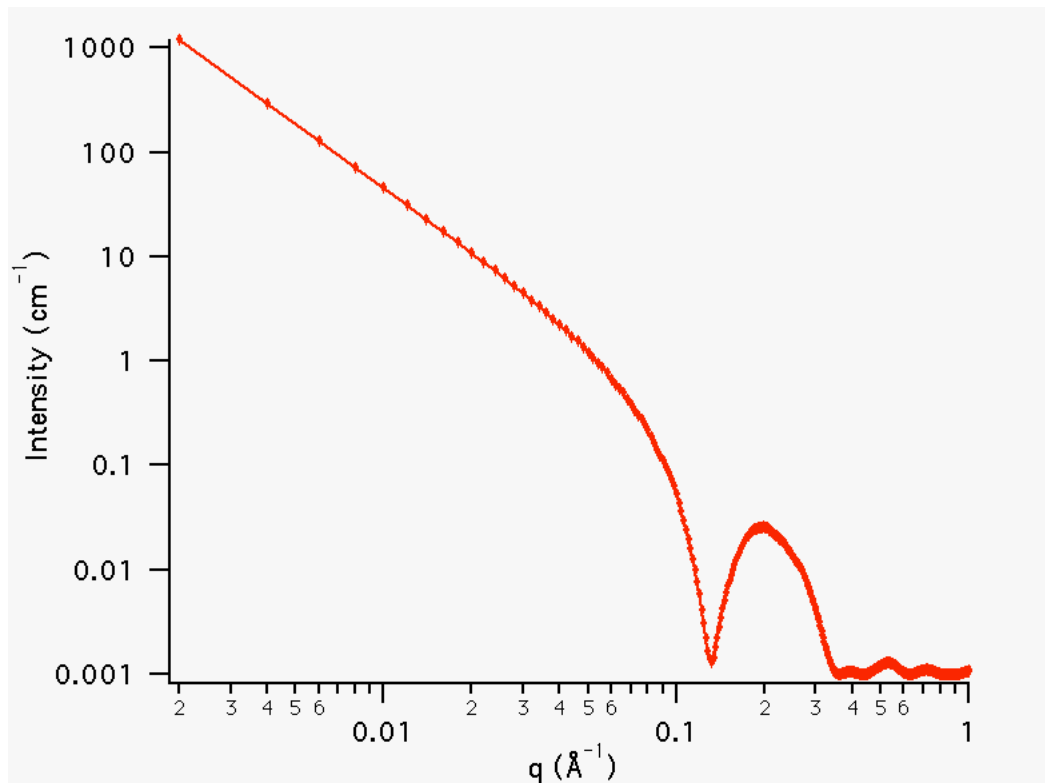
Guinier, A. and Fournet, G., "Small-Angle Scattering of X-Rays", John Wiley and Sons, New York, 1955.

Kratky, O. and Porod, G., J. Colloid Science, 4, 35, 1949.

Higgins, J.S. and Benoit, H.C., "Polymers and Neutron Scattering", Clarendon, Oxford, 1994.

## TEST DATASET

This example dataset is produced by running the Macro PlotStackedDiscs(), using 500 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 1.0 \text{ \AA}^{-1}$  and the above default coef\_scyl values.



## • Structure Factors for Interacting Particles

### Hard Sphere Structure Factor

#### MACRO : FUNCTION

PlotHardSphereStruct() : HardSphereStruct(w,y,x)

Wave extension: \_hss

File:

HardSphereStruct.ipf

Requires:

none

**AUTHOR/MODIFICATION**

Steve Kline 06 NOV 1998

**APPROVED FOR DISTRIBUTION**

Sungmin Choi 02 FEB 199

**DESCRIPTION**

Calculates the interparticle structure factor for monodisperse spherical particles interacting through hard sphere (excluded volume) interactions. The solution uses the Percus-Yevick closure.

**VARIABLES**

Input Variables (default values):

Point	parameters_hss	coef_hss
0	Radius (A)	50
1	vol fraction	0.2

**USAGE NOTES**

The returned value is dimensionless

The interparticle potential is:

$$U(r) = \begin{cases} \infty & r < 2R \\ 0 & r \geq 2R \end{cases}$$

where  $r$  is the radial distance from the center of the sphere of radius  $R$ .

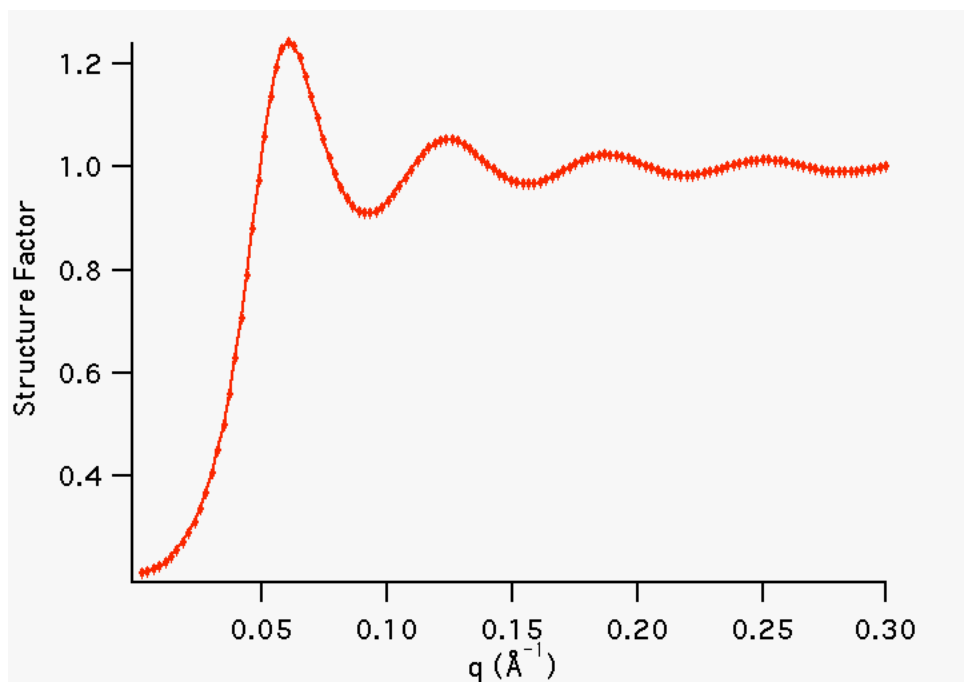
No intraparticle (form factor) scattering is included.

**REFERENCE**

Percus, J. K.; Yevick, G. *J. Phys. Rev.* **1958**, *110*, 1.

**TEST DATASET**

This example dataset is produced by running the Macro PlotHardSphereStruct(), using 128 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.3 \text{ \AA}^{-1}$  and the above default coef\_hss values.



### Square Well Structure Factor

#### **MACRO : FUNCTION**

PlotSquareWellStruct() : SquareWellStruct(w,y,x)

Wave extension:     \_sws

File:

[SquareWellStruct.ipf](#)

Requires:

none

#### **AUTHOR/MODIFICATION**

Steve Kline   06 NOV 1998

#### **APPROVED FOR DISTRIBUTION**

Sungmin Choi 02 FEB 1999

#### **DESCRIPTION**

Calculates the interparticle structure factor for a square well fluid of spherical particles.

#### **VARIABLES**

Input Variables (default values):

Point	parameters_sws	coef_sws
0	Radius (A)	50
1	vol fraction	0.04
2	well depth (kT)	1.5
3	well width (diameters)	1.2

## USAGE NOTES

The returned value is dimensionless.

The mean spherical approximation (MSA) closure was used for this calculation, and is not the most appropriate closure for an attractive interparticle potential. This solution has been compared to Monte Carlo simulations for a square well fluid, showing this calculation to be limited in applicability to well depths  $\varepsilon < 1.5$  kT and volume fractions  $\phi < 0.08$ .

Positive well depths correspond to an attractive potential well. Negative well depths correspond to a potential "shoulder", which may or may not be physically reasonable.

The well width ( $\lambda$ ) is defined as multiples of the particle diameter ( $2R$ )

The interaction potential is:

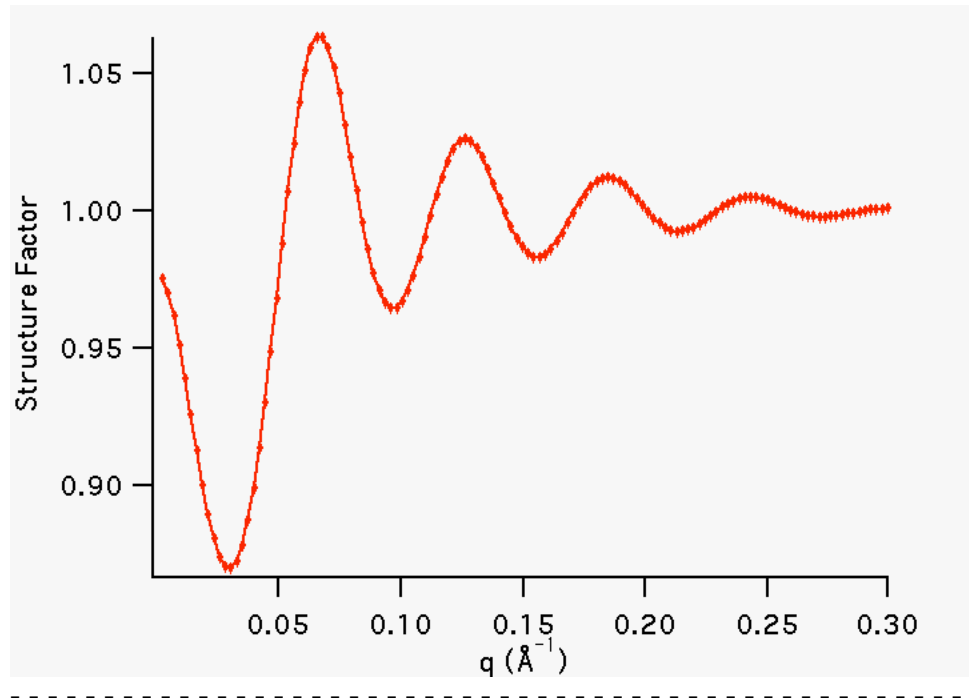
$$U(r) = \begin{cases} \infty & r < 2R \\ -\varepsilon & 2R \leq r \leq 2R\lambda \\ 0 & r > 2R\lambda \end{cases}$$

## REFERENCE

Sharma, R. V.; Sharma, K. C. *Physica*, **1977**, *89A*, 213.

## TEST DATASET

This example dataset is produced by running the Macro PlotSquareWellStruct(), using 128 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.3 \text{ \AA}^{-1}$  and the above default coef\_sws values.



## Screened Coulomb Structure Factor

### MACRO : FUNCTION

PlotHayterPenfoldMSA() : HayterPenfoldMSA(w,y,x)

Wave extension:       \_hpmsa

File:

HPMSA.ipf

Requires:

PlotUtils.ipf

### AUTHOR/MODIFICATION

Paul Butler    14 NOV 1999

### APPROVED FOR DISTRIBUTION

S. Kline        17 NOV 1999

### DESCRIPTION

Calculates the Structure factor (the Fourier transform of the pair correlation function  $g(r)$ ) for a system of charged, spheroidal objects in a dielectric medium. When combined with an appropriate form factor (such as sphere, core+shell, ellipsoid etc..), this allows for inclusion of the interparticle interference effects due to screened coulomb repulsion between charged particles.

### VARIABLES

Input Variables (default values):

Point	parameters_hpmsa	coef_hpmsa
0	Diameter (A)	41.5
1	Charge	19
2	Volume Fraction	0.0192
3	Temperature(K)	318.16
4	monovalent salt conc. (M)	0
5	dielectric constant of solvent	71.08

### USAGE NOTES

This routine only works for charged particles. If w[1] (the charge) is set to zero the routine will self destruct. For non-charged particles use a hard sphere potential.

w[4], the salt concentration, is used to compute the ionic strength of the solution which in turn is used to compute the Debye screening length. At present there is no provision for entering the ionic strength directly nor for use of any multivalent salts. The counterions are also assumed to be monovalent.

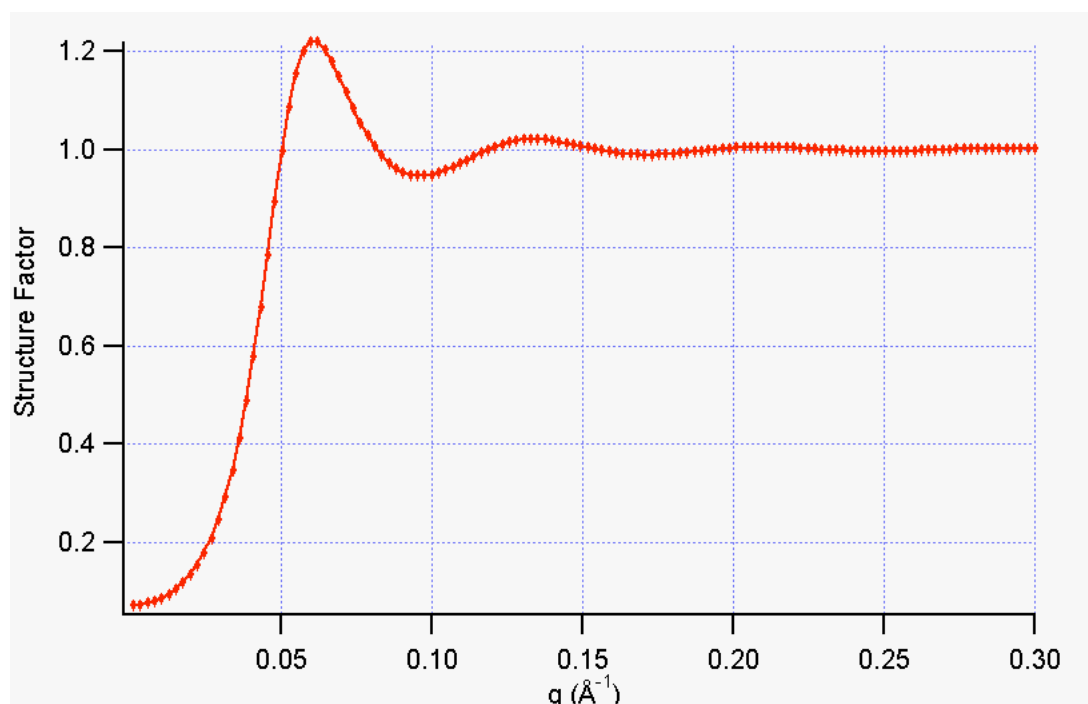
### REFERENCE

1. JP Hansen and JB Hayter "A rescaled MSA structure factor for dilute charged colloidal dispersions" Molecular Physics **46**, 651-656 (1982).

2. JB Hayter and J Penfold "An analytic structure factor for macroion solutions" Molecular Physics **42**, 109-118 (1981).

## TEST DATASET

This example dataset is produced by running the Macro PlotHayterPenfoldMSA(), using 128 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.3 \text{ (\AA}^{-1})$  and the above default coef\_hpmsa values.



## Sticky Hard Sphere Structure Factor

### MACRO : FUNCTION

Plot\_StickyHS\_Struct() : StickyHS\_Struct(w,y,x)

Wave extension : \_shsSQ

File:

StickyHardSphereStruct.ipf

Requires:

none

### AUTHOR/MODIFICATION

Steve Kline 14 JUL 2004

### APPROVED FOR DISTRIBUTION

WeiRen Chen 01 FEB 2006

### DESCRIPTION

Calculates the interparticle structure factor for a hard sphere fluid with a narrow attractive well. A perturbative solution of the Percus-Yevick closure is used. The strength of the attractive well is described in terms of "stickiness" as defined below.

### VARIABLES

Input Variables (default values):



Point	parameters_shsSQ	coef_shsSQ
0	Radius	50
1	volume fraction	0.1
2	perturbation parameter (0.1)	0.05
3	stickiness, tau	0.2

## USAGE NOTES

The returned value is a dimensionless structure factor,  $S(q)$ .

The perturbation parameter, epsilon, should be held between 0.01 and 0.1. It is best to hold the perturbation parameter fixed and let the "stickiness" vary to adjust the interaction strength. The stickiness, tau, is defined in equation 21 and is a function of both the perturbation parameter and the interaction strength. Tau and epsilon are defined in terms of the hard sphere diameter ( $\sigma = 2R$ ), the width of the square well,  $\Delta$  (same units as  $R$ ), and the depth of the well,  $u_o$ , in units of  $kT$ . From the definition, it is clear that smaller tau mean stronger attraction.

$$\tau = \frac{1}{12\epsilon} \exp(u_o / kT)$$

$$\epsilon = \Delta / (\sigma + \Delta)$$

The interaction potential is:

$$u(r) = \begin{cases} \infty & r < \sigma \\ -u_o & \sigma < r < \sigma + \Delta \\ 0 & r > \sigma + \Delta \end{cases}$$

The Percus-Yevick (PY) closure was used for this calculation, and is an adequate closure for an attractive interparticle potential. This solution has been compared to Monte Carlo simulations for a square well fluid, with good agreement.

The true particle volume fraction,  $\phi$ , is not equal to  $\eta$ , which appears in most of the reference. The two are related in equation (24) of the reference. The reference also describes the relationship between this perturbation solution and the original sticky hard sphere (or adhesive sphere) model by Baxter.

NOTES: The calculation can go haywire for certain combinations of the input parameters, producing unphysical solutions - in this case errors are reported to the command window and the  $S(q)$  is set to -1 (it will disappear on a log-log plot). Use tight bounds to keep the parameters to values that you know are physical (test them) and keep nudging them until the optimization does not hit the constraints.

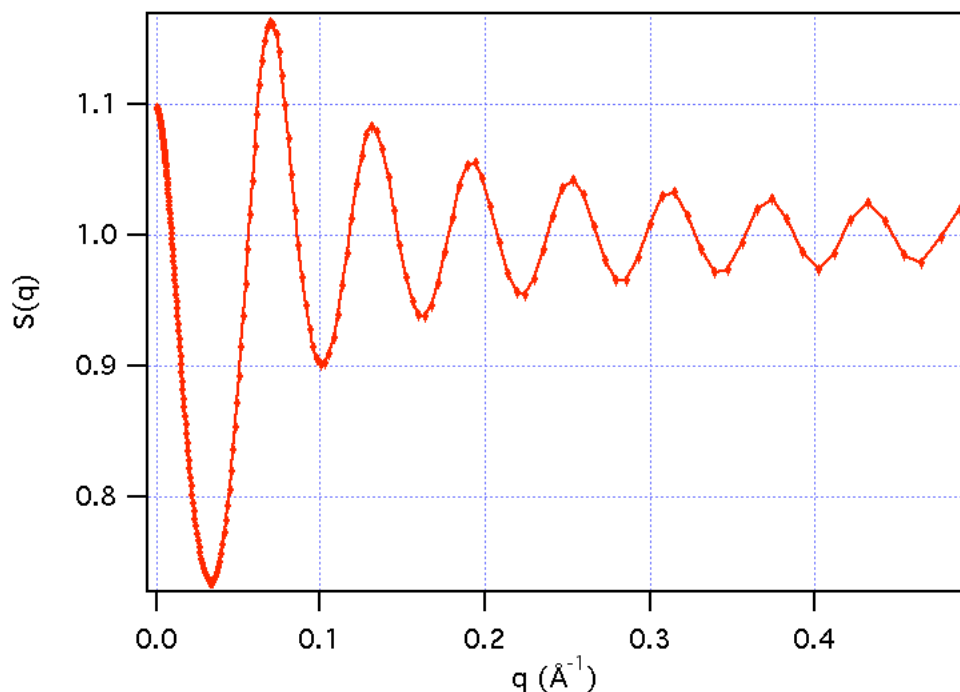
## REFERENCE

Menon, S. V. G., Manohar, C. and K. Srinivas Rao *J. Chem. Phys.*, **1991**, *95*(12), 9186-9190. Note that in this reference equation (23) should read:

$$\lambda\tau = \frac{(1+\eta/2)}{(1-\eta)^2} - \frac{\lambda\eta}{(1-\eta)} + \frac{\lambda^2\eta}{12} + O(\varepsilon)$$

### TEST DATASET

This example dataset is produced by running the Macro Plot\_StickyHS\_Struct(), using 256 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.5 \text{ \AA}^{-1}$  and the above default coef\_shsSQ values.



## • Interacting Particles

### Polydisperse Hard Spheres

#### MACRO : FUNCTION

PlotPolyHardSpheres() : PolyHSIntensity(w,y,x)

Wave extension : \_phs

File:

PolyHardSphereInten.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

#### AUTHOR/MODIFICATION

**APPROVED FOR DISTRIBUTION**

Sungmin Choi 02 FEB 1999

**DESCRIPTION**

This function calculates the scattered intensity for a population of polydisperse spheres, including hard sphere interactions between the particles. The calculation is an exact, multicomponent solution, using the Percus-Yevick closure. A Schulz distribution is used to describe the polydispersity of the diameter. Partial structure factors are calculated for the size distribution. No monodisperse structure factor approximations are used in this solution

**VARIABLES**

Input Variables (default values):

parameters_phs	coef_phs
Radius (A)	100
polydispersity	0.12
volume fraction	0.1
SLD sphere (A <sup>-2</sup> )	1e-06
SLD solvent (A <sup>-2</sup> )	6.3e-06
background (cm <sup>-1</sup> )	0.1

**USAGE NOTES**

The function calculates the scattered intensity from a polydisperse population of spheres of uniform scattering length density. The results are applicable to any PHS fluid which can be represented by a Schulz distribution. The partial structure factors of the different sized particles is accounted for rigorously in the Percus-Yevick closure approximation, one which has been shown through simulation to be very good for even dense hard sphere fluids. This analytic expression for the scattered intensity avoids the approximations caused by factoring the expressions for polydisperse systems to allow (sometimes VERY) approximate monodisperse structure factors to be used to (approximately) describe a polydisperse HS fluid. If PHS applies to your system, use this functional form over any approximation.

What is calculated is:

$$I(q) = n \int_0^\infty F_i^2(q) f(\sigma_i) d\sigma_i \\ + n \int_0^\infty \int_0^\infty F_i(q) F_j(q) H_{ij}(q) f_i(\sigma_i) f_j(\sigma_j) d\sigma_i d\sigma_j$$

where

$$H_{ij}(q) = S_{ij}(q) - 1$$

are the partial structure functions, related to the partial structure factors,  $S_{ij}(q)$ . The full equations can be found in the reference.

The returned value is the scattered intensity in absolute scale, units of [cm<sup>-1</sup>].

Polydispersity,  $p = \sigma/R$ , where  $\sigma^2$  is the variance of the distribution and  $R$  is the mean particle radius, `coef_phs[0]`. For a more complete description of the Schulz distribution, see: J. Hayter in "Physics of Amphiphiles - Micelles, Vesicles and Microemulsions" V. DeGiorgio and M. Corti, Eds. (1983) p. 69.

Polydispersity, `w[1]`, often needs to be constrained during fitting to remain between its physical limits of  $0 < p < 1$ .

Scattering contrast = SLD (sphere) - SLD (solvent).

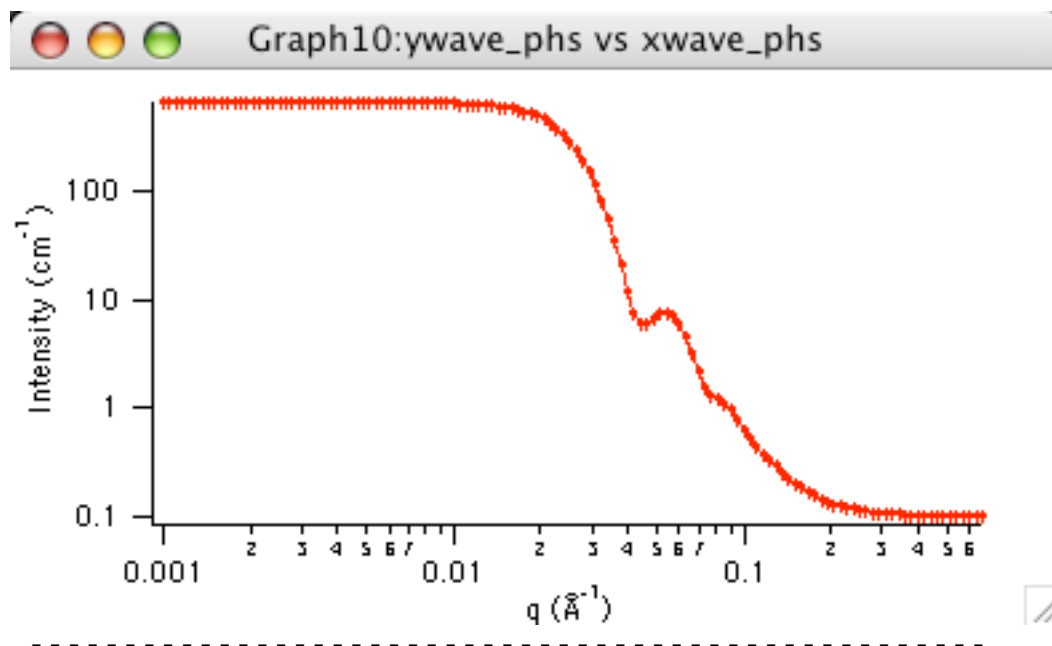
Volume fraction and scattering contrast are correlated, and one or both should be held fixed during model fitting.

## REFERENCE

Griffith, W. L.; Triolo, R.; Compere, A. L. *Phys. Rev. A*, **1987**, 35, 2200.

## TEST DATASET

This example dataset is produced by running the `Macro PlotPolyHardSpheres()`, using 256 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.7 \text{ \AA}^{-1}$  and the above default `coef_phs` values.



## Binary Hard Spheres

### MACRO : FUNCTION

`Plot_BinaryHS()` : `BinaryHS(w,y,x)`

`Plot_BinaryHS_PSF()`

`Calculate_BHS_Parameters()`

`Duplicate_AL_Parameters()`

Wave extension :     \_binaryHS  
File:                    BinaryHardSpheres.ipf  
Requires:               GaussUtils.ipf  
                          PlotUtils.ipf

**AUTHOR/MODIFICATION**  
Steve Kline   14 JUL 2004

**APPROVED FOR DISTRIBUTION**  
WeiRen Chen  01 FEB 2006

## DESCRIPTION

This function calculates the scattered intensity for a binary mixture of spheres, including hard sphere interactions between the particles. Both of the populations are monodisperse. The calculation is an exact, multicomponent solution, using the Percus-Yevick closure. The three partial structure factors can also be calculated through a separate macro. A resolution smeared version of the scattered intensity is provided.

## VARIABLES

Input Variables (default values):

Point	parameters_BinaryHS	coef_BinaryHS
0	large radius	100
1	small radius	25
2	volume fraction large spheres	0.2
3	volume fraction small spheres	0.1
4	large sphere SLD	3.5e-06
5	small sphere SLD	5e-07
6	solvent SLD	6.36e-06
7	Incoherent Bgd (cm-1)	0.001

## USAGE NOTES

The function that is calculated is the total scattered intensity from the binary mixture in absolute scale, units of [cm<sup>-1</sup>]. The calculation is exact in the Percus-Yevick closure.

$$I(q) = (1-x) f_1^2(q) S_{11}(q) + 2[x(1-x)]^{1/2} f_1(q) f_2(q) S_{12}(q) \\ + x f_2^2(q) S_{22}(q)$$

where the  $S_{ij}(q)$  are the partial structure factors, the  $f_i(q)$  are the scattering amplitudes of the spherical particles. The subscript (1) is the smaller sphere, and (2) is the larger sphere.  $x$  is the number fraction of larger spheres, and is defined as:

$$x = \frac{n_2}{n_1 + n_2}$$

with  $n$  being the number density of each population of spheres. The number fraction,  $x$ ,

is automatically calculated based on the diameter ratio and the volume fractions as:

$$x = \frac{(\phi_2 / \phi) \alpha^3}{(1 - (\phi_2 / \phi) + (\phi_2 / \phi) \alpha^3)}$$

where the total volume fraction and size ratio are defined as in the original reference:

$$\phi = \phi_1 + \phi_2$$

$$\alpha = R_1 / R_2$$

The number fraction can be calculated by the supplied macro as described below.

Notes:

The volume fractions and the scattering contrasts are loosely correlated (in a complex way), so holding as many parameters fixed to known values during fitting will improve the robustness of the fit.

Since the calculation uses the Percus-Yevick closure, all of the limitations of that closure relation apply here. Specifically, one should be wary of results for (total) volume fractions greater than approximately 40%. Depending on size ratios or number fractions, the limit on total volume fraction may be lower.

## Macros:

### Plot\_BinaryHS\_PSF()

Plots the three partial structure factors versus  $Q \cdot R_2^2$  (the wave QD2\_BinaryHS). The partial structure factors can also be plotted against  $q$  (the wave xwave\_BinaryHS) just like the total intensity.

### Calculate\_BHS\_Parameters()

This macro will take the radii and volume fractions in the coef\_BinaryHS wave and calculate the number fractions of each component.

### Duplicate\_AL\_Parameters()

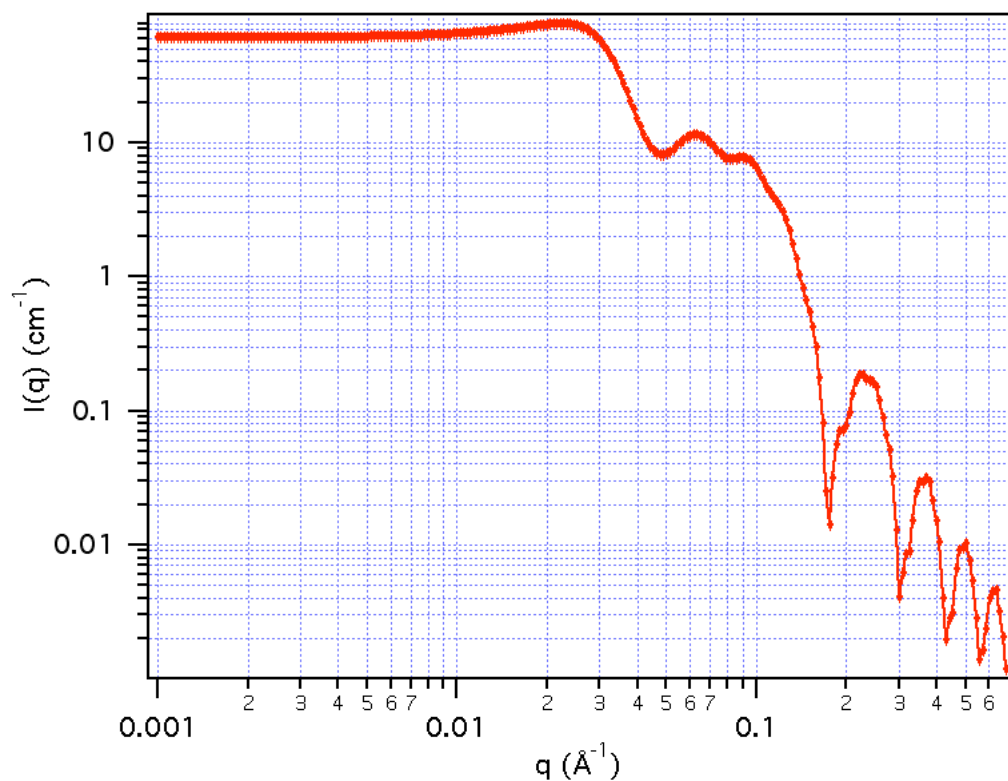
This macro takes as input  $\eta$ ,  $x$ , and  $\alpha$  as defined in Ashcroft and Lagreth's (AL) paper. It also takes an actual radius of the larger sphere (in Angstroms). These values are converted into radii and volume fractions, and automatically copied to the coef\_BinaryHS wave. Intensity or PSF graphs that are open will automatically update. This is particularly useful for duplicating the figures in the AL paper.

## REFERENCE

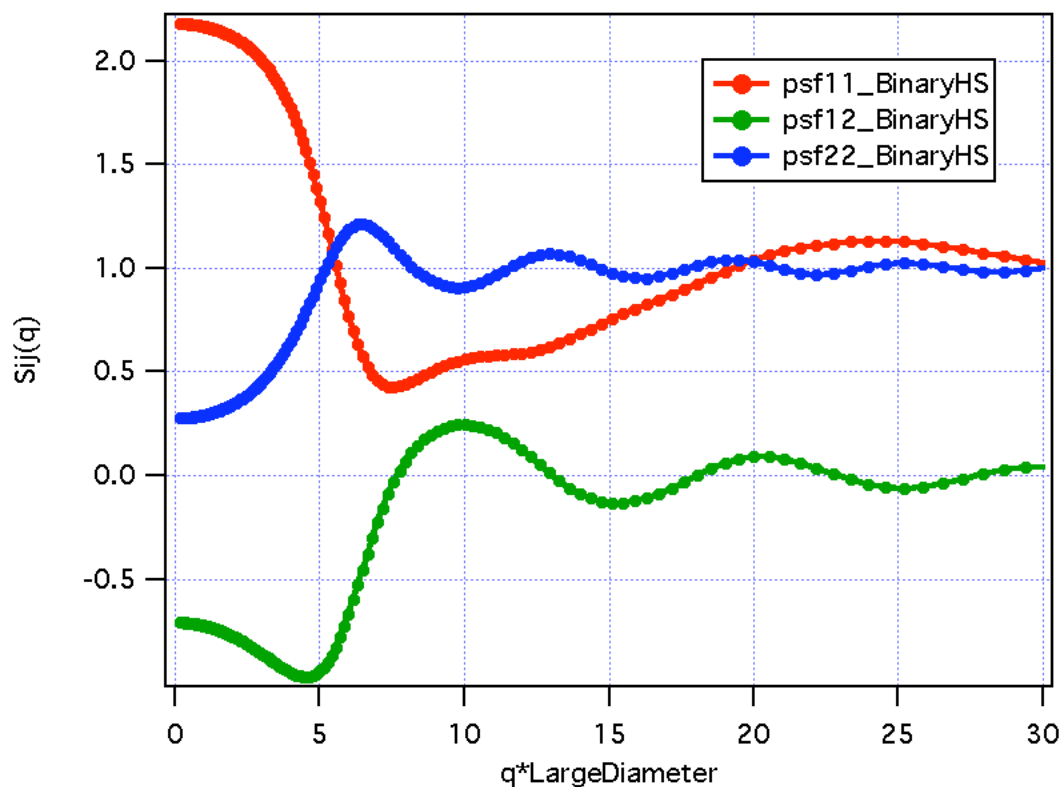
N. W. Ashcroft and D. C. Langreth, Physical Review, v. 156 (1967) 685-692.  
[Errata found in Phys. Rev. 166 (1968) 934.]

## TEST DATASET

This example dataset is produced by running the Macro Plot\_BinaryHS(), using 256 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_BinaryHS values.



The three partial structure factors that are combined to generate the total scattering can be generated by using the macro `Plot_BinaryHS_PSF()`. These partial structure factors are dependent on the `coef_BinaryHS` and will change as those coefficients are changed. They are automatically plotted against the wave `QD2_BinaryHS` which is  $Q \cdot R_{\text{large}} \cdot 2$ , giving a dimensionless x-axis. This is for direct comparison to the figures given in the original reference. The partial structure factors can also be plotted versus the `xwave_BinaryHS`. The macro defaults to plot the scaled x-axis over a range of (0,30) for clarity.



## • Polymer Models

### Debye Model

#### **MACRO : FUNCTION**

PlotDebye() : Debye(w,y,x)

Wave extension: \_deb

File:

Debye.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

#### **AUTHOR/MODIFICATION**

Steve Kline 06 NOV 1998

#### **APPROVED FOR DISTRIBUTION**

Charlie Glinka 06 SEP 2003

#### **DESCRIPTION**

Calculates the Debye function,  $D(x)$ ,

$$D(x) = 2(e^{-x} + x - 1)/x^2 \quad x = (qR_g)^2$$

$D(x)$  represents the form factor for a linear polymer chain in the melt or in dilute



solution (theta solvent). In addition to the radius of gyration,  $R_g$ , a scale factor "scale", and a constant background term are included in the calculation. The macroscopic scattering cross section for this model is, therefore,

$$d\Sigma/d\Omega = scale * D(x) + bkg$$

For a dilute solution of polymer chains in a theta solvent,

$$scale = \phi (\Delta\rho)^2 Z v_m$$

$\phi$  = polymer volume fraction

$\Delta\rho$  = scattering contrast

$Z$  = number of monomers per chain

and  $v_m$  = volume of a monomer

Resolution smeared version is also provided.

## VARIABLES

Input Variables (default values):

Point	parameters_deb	coef_deb
0	scale	1
1	$R_g$ (Å)	50
2	bkg (cm <sup>-1</sup> )	0.001

## USAGE NOTES

The returned value is scaled to units of [cm<sup>-1</sup>]

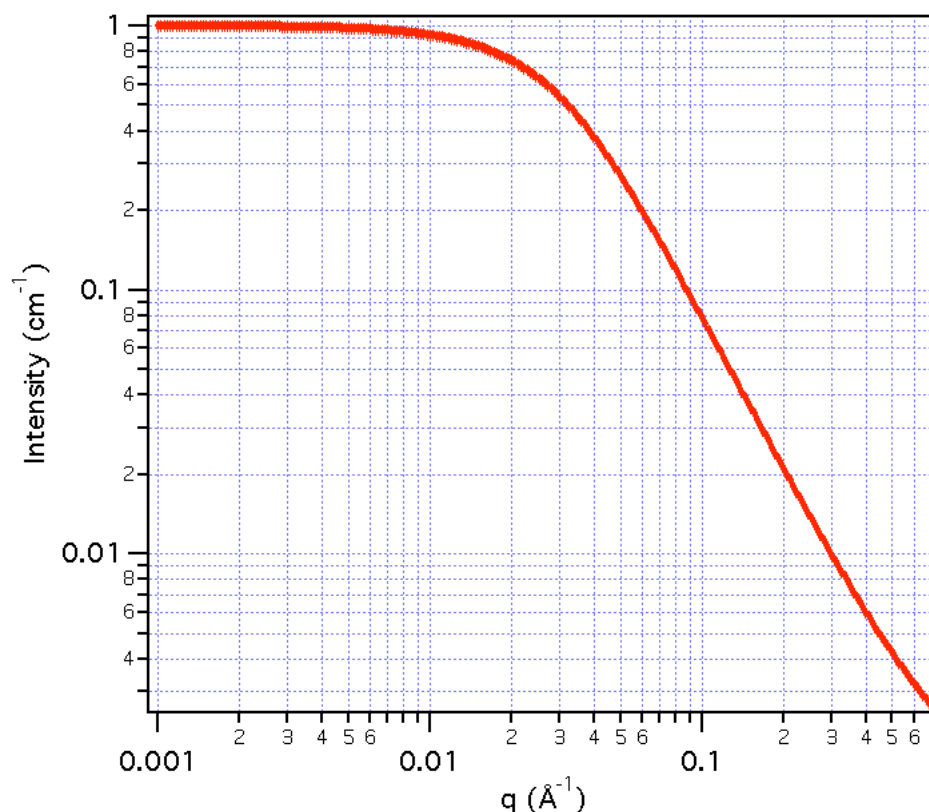
Scattering contrast = SLD (polymer) - SLD (solvent)

## REFERENCE

Roe, R.-J., "Methods of X-Ray and Neutron Scattering in Polymer Science", Oxford University Press, New York, (2000).

## TEST DATASET

This example dataset is produced by running the Macro PlotDebye(), using 128 data points,  $q_{min} = 0.001 \text{ Å}^{-1}$ ,  $q_{max} = 0.3 \text{ (Å}^{-1})$  and the above default coef\_deb values.



## RPA - 10 cases

### MACRO : FUNCTION

PlotRPAForm() : RPAForm(w,y,x)

Wave extension: \_rpa

File:

SmearedRPA.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

### AUTHOR/MODIFICATION

B. Hammouda 21 JAN 1999

### APPROVED FOR DISTRIBUTION

S. Kline 22 JAN 1999

### DESCRIPTION

Calculates the macroscopic scattering intensity (units of cm<sup>-1</sup>) for a multicomponent homogeneous mixture of polymers using the Random Phase Approximation. This general formalism contains 10 specific cases:

Case 1: C/D Binary mixture of homopolymers

Case 2: C-D Diblock copolymer

Case 3: B/C/D Ternary mixture of homopolymers

Case 4: C/C-D Mixture of a homopolymer B and a diblock copolymer C-D

Case 5: B-C-D Triblock copolymer  
Case 6: A/B/C/D Quaternary mixture of homopolymers  
Case 7: A/B/C-D Mixture of two homopolymers A/B and a diblock C-D  
Case 8: A/B-C-D Mixture of a homopolymer A and a triblock B-C-D  
Case 9: A-B/C-D Mixture of two diblock copolymers A-B and C-D  
Case 10: A-B-C-D Four-block copolymer  
Resolution smeared version is also provided.

## VARIABLES

Fitting Parameters (default values):

Point	coefnames_rpa	coefvalues_rpa
0	Seg. Length bc	5
1	Seg. Length bd	5
2	Chi Param. Kcd	-0.0004
3	scale	1

Fixed Input Parameters (default values):

Point	inputnames	inputvalues
0	Deg. Polym. Nc	1000
1	Vol. Frac. Phic	0.5
2	Spec. Vol. Vc	100
3	Scatt. Length Lc	1e-12
4	Deg. Polym. Nd	1000
5	Vol. Frac. Phid	0.5
6	Spec. Vol. Vd	100
7	Scatt. LengthLd	0

## USAGE NOTES

Only one case can be used at any one time. Plotting a different case will overwrite the original parameter waves.

The returned value is scaled to units of  $[\text{cm}^{-1}]$ .

Component D is assumed to be the "background" component (all contrasts are calculated with respect to component D).

Scattering contrast for a C/D blend=  $\{\text{SLD (component C)} - \text{SLD (component D)}\}^2$

Depending on what case is used, the number of fitting parameters (w[0], w[1], w[2], etc) varies. These represent the segment lengths (ba, bb, etc) and the Chi parameters (Kab, Kac, etc). The last one of these is a scaling factor to be held constant equal to unity. The input parameters are the degree of polymerization (var[0], var[4], etc), the volume fractions for each component (var[1], var[5], etc) the specific volumes (var[2], var[6], etc) and the neutron scattering length densities (var[3], var[7], etc).

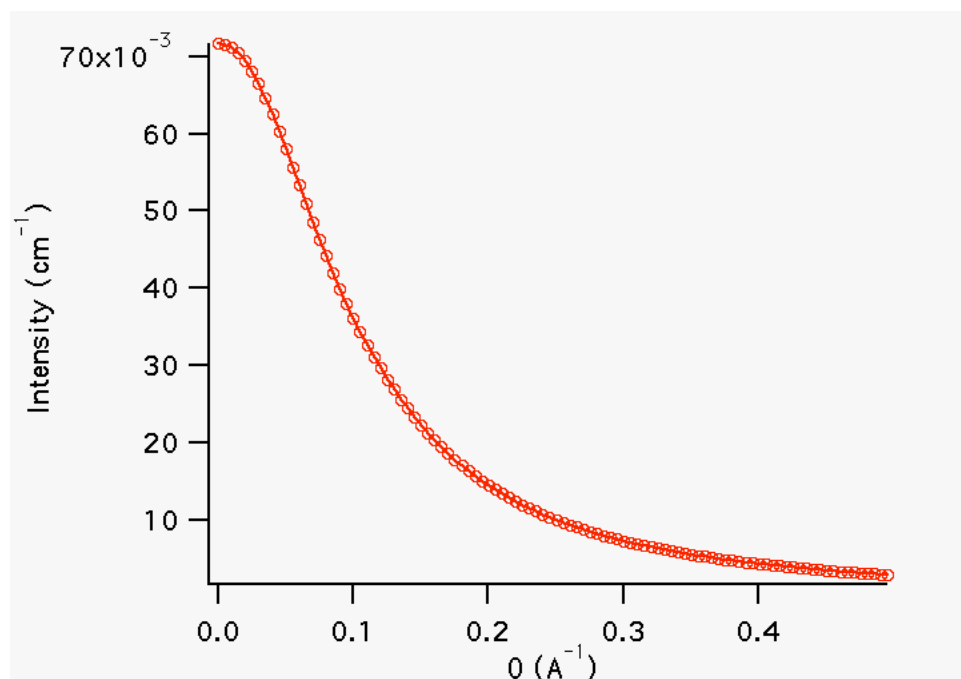
This RPA (mean field) formalism applies only when the multicomponent polymer mixture is in the homogeneous mixed-phase region.

## REFERENCE

A.Z. Akcasu, R. Klein and B. Hammouda, Macromolecules 26, 4136 (1993)

## TEST DATASET

This example dataset is produced by running the Macro PlotRPAForm() for CASE 1, using 100 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.5 \text{ (\AA}^{-1})$  and the above default fitting and input parameter values.



---

## Polyelectrolyte - Borue

### MACRO : FUNCTION

PlotBE\_Polyelectrolyte() : BEPolyelectrolyte(w,y,x)

Wave extension: \_BE

File:

BE\_Polyelectrolyte.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

### AUTHOR/MODIFICATION

Giovanni Nisato 30 NOV 1998

### APPROVED FOR DISTRIBUTION

Steve Kline 07 DEC 1998

## DESCRIPTION

Calculates the structure factor of a polyelectrolyte solution with the RPA expression derived by Borue and Erukhimovich.

Resolution smeared version is also provided.

## VARIABLES

Input Variables (default values):

Point	parameters_BE	coef_BE
0	K (barns)	10
1	Lb (Å)	7.1
2	h (Å <sup>-3</sup> )	12
3	b (Å)	10
4	Cs (mol/L)	0
5	alpha	0.05
6	C (mol/L)	0.7
7	Background	0.001

## USAGE NOTES

The returned value is scaled to units of [cm<sup>-1</sup>]

K = contrast factor of the polymer (barns = 10<sup>-24</sup> cm<sup>2</sup>)

NB:  $K = a^2$  with:  $a = (b_p - v_p/v_{\text{solvent}} * b_{\text{solvent}})$

where: b = Sum of the scattering lengths of the atoms constituting the Monomer of the polymer under consideration.

$v_p$  = partial molar volume of the polymer ;

$v_{\text{solvent}}$  = partial molar volume of the solvent

Lb = Bjerrum length(Å)

Nb: This parameter needs to be kept constant for a given solvent and temperature!

h = virial parameter (Å<sup>3</sup>)

NB : See (1) for the correct interpretation of this parameter. It incorporates second and third virial coefficients and can be Negative

b = monomer length (Å)

Cs = concentration of monovalent salt (mol/L)

Alpha = ionization degree : ratio of charged monomers to total number of monomers

C = polymer molar concentration (mol/L)

Bkd = Background

The fitting procedure does not follow the notation of (1) since the two parameters 's' and 't' are NOT decoupled.

The following expression is used instead:

$$S_q = K \cdot 1. / (4 \cdot \pi \cdot L_b \cdot \alpha^2) \cdot (q^2 + k^2) / (1 + (r_0^2 \cdot q^2) \cdot (q^2 + k^2) \cdot (q^2 - (12 \cdot h \cdot C / b^2))) + B_{kd}$$

The procedure fits the data using the following internal parameter:

$$k^2 = 4 \cdot \pi \cdot L_b \cdot (2 \cdot C_s + \alpha \cdot C)$$

which corresponds to the classical definition of the inverse Debye length, squared.

An alternative definition for for ANNEALED (weak) polyelectrolytes (e.g. : polyacrylic acid) is given by (4):

$$k^2 = 4 \cdot \pi \cdot L_b \cdot (2 \cdot C_s + 2 \cdot \alpha \cdot C_a)$$

## REFERENCE

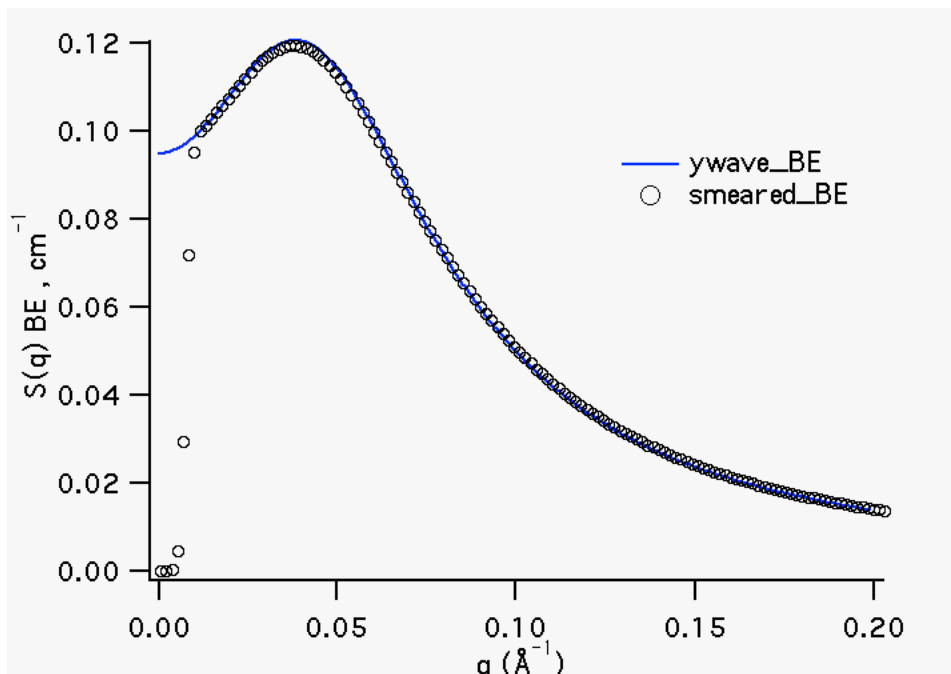
- 1) Borue, V. Y.; Erukhimovich, I. Y. Macromolecules 1988, 21, 3240.
- 2) Joanny, J.-F.; Leibler, L. Journal de Physique 1990, 51, 545.
- 3) Moussaid, A.; Schosseler, F.; Munch, J.-P.; Candau, S. J. Journal de Physique II France 1993, 3, 573.
- 4) Raphaël, E.; Joanny, J.-F. Europhysics Letters 1990, 11, 179.

## TEST DATASET

This example dataset is produced by running the Macros:

- \* PlotBE(), using 512 data points,  $q_{min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{max} = 0.2 \text{ (\AA}^{-1})$  and the above default coef\_BE values.
- \* PlotSmearedBE(), using the QSIG\_4M\_22.AVE data set for the smeared q values and the above default coef\_BE values.

It reproduces the results found in reference (3).



## • Two-Phase Structures

## Lorentz

### MACRO : FUNCTION

Plot\_Lorentz() : Lorentz(w,y,x)

Wave extension: \_Lorentz

File:

Lorentz\_model.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

### AUTHOR/MODIFICATION

John Barker 22 FEB 1999

### APPROVED FOR DISTRIBUTION

Steve Kline 24 FEB 1999

### DESCRIPTION

Model describes a Lorentzian (Ornstein-Zernicke) including a flat background,

$$I(q) = I_0 / [ 1 + \{qL\}^2 ] + \text{BGD}$$

with screening length L. The parameters  $I_0$ , L, and BGD can all be adjusted during fitting.

Resolution smeared version is also provided.

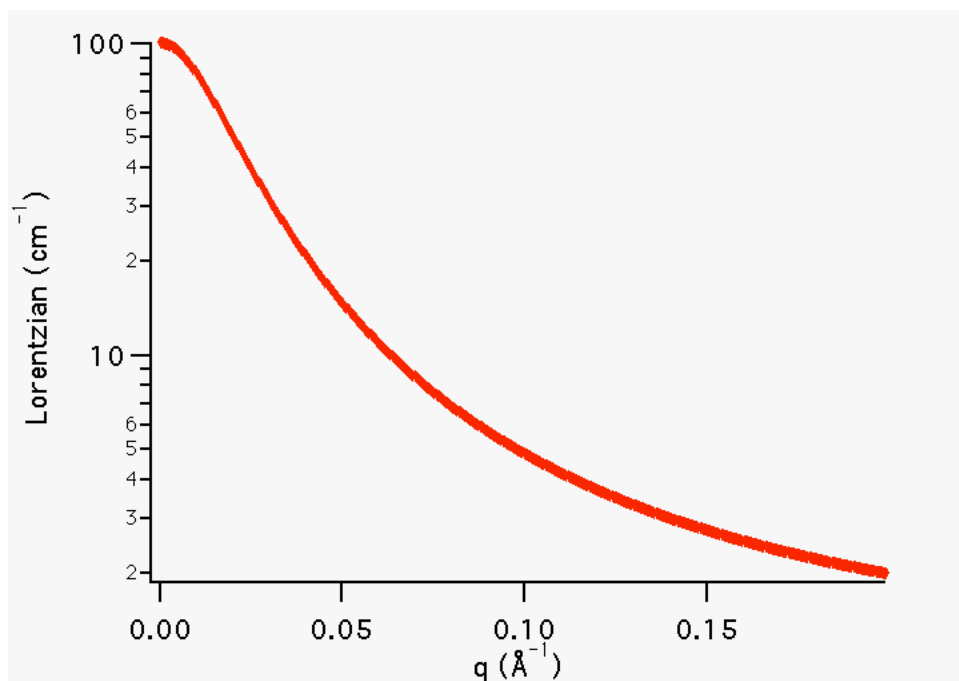
### VARIABLES

Input Variables (default values):

Point	parameters_Lorentz	coef_Lorentz
0	Scale Factor, $I_0$	100
1	Screening Length ( $\text{\AA}$ )	50
2	Incoherent Bgd ( $\text{cm}^{-1}$ )	1

### TEST DATASET

This example dataset is produced by the Macro Plot\_Lorentz() using the default parameter values given above. The q-range has been restricted to  $(0.001, 0.2) \text{ \AA}^{-1}$ .



### Debye-Anderson-Brumberger

#### **MACRO : FUNCTION**

PlotDAB() : DAB\_Model(w,y,x)

Wave extension: \_DAB

File:

DAB\_model.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

#### **AUTHOR/MODIFICATION**

Charlie Glinka 5 DEC 1998

#### **APPROVED FOR DISTRIBUTION**

Steve Kline 4 JAN 1999

#### **DESCRIPTION**

Calculates the scattering from a randomly distributed (i.e. nonparticulate), two-phase system based on the Debye-Anderson-Brumberger (DAB) model for such systems. The two-phase system is characterized by a single length scale, the correlation length, which is a measure of the average spacing between regions of phase 1 and phase 2. The model also assumes smooth interfaces between the phases and hence exhibits Porod behavior ( $I \sim Q^{-4}$ ) at large  $Q$  ( $Q \cdot \text{correlation length} \gg 1$ ). The macroscopic scattering cross-section in the DBA model is given by

$$d\Sigma/d\Omega = A/(1 + (q \cdot a)^2)^{3/2}$$

where  $a$  is the correlation length in Å.



Resolution smeared version is also provided.

## VARIABLES

Input Variables (default values):

Point	parameters_DAB	coef_DAB
0	Scale Factor, A	10
1	Correlation Length (Å)	40
2	Incoherent Bgd (cm <sup>-1</sup> )	1

## USAGE NOTES

The returned value is in units of [cm<sup>-1</sup>].

The scale factor, A or w[0], is treated as an independent fitting parameter, but is, in the DBA model, related to the volume fractions of the two phases,  $\phi_1$  and  $\phi_2$ , their contrast,  $(sld_1 - sld_2)^2$ , and the correlation length, a, as follows:

$$A = 8\pi a^3 \text{contrast} \phi_1 \phi_2$$

The surface, S, to volume, V, ratio for the system is given by

$$S/V = 4\phi_1\phi_2 / a$$

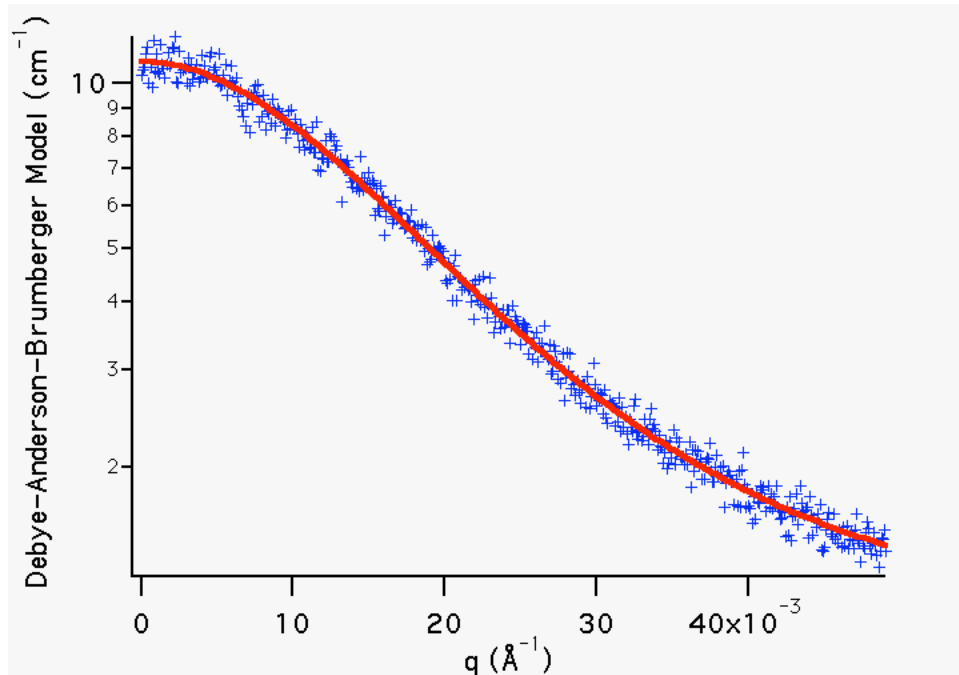
## REFERENCES

Debye, P., Anderson, R., Brumberger, H., "Scattering by an Inhomogeneous Solid. II. The Correlation Function and Its Application," J. Appl. Phys. **28** (6), 679 (1957).

Debye, P., Bueche, A. M., "Scattering by an Inhomogeneous Solid," J. Appl. Phys. **20**, 518 (1949).

## TEST DATASET

This example dataset is produced by multiplying the values generated by the Macro PlotDAB() (using the default parameter values given above) by  $(1 + \text{gnoise}(.05))$  to simulate real data with 5% gaussian noise. The q-range has been restricted to (0.001,0.05) Å<sup>-1</sup>. The weighting wave was set to  $1/\sqrt{y_{\text{wave\_DAB}}}$  at the default coefficient values.



Starting values for test fit:

Point	parameters_DAB	coef_DAB
0	Scale Factor, A	10
1	Correlation Length (Å)	40
2	Incoherent Bgd (cm <sup>-1</sup> )	1

Fitted values and standard deviations

Sum of squares = 6.58442

Point	parameters_DAB	coef_DAB	W_sigma
0	Scale Factor, A	9.94365	0.351635
1	Correlation Length (Å)	39.8374	2.19435
2	Incoherent Bgd (cm <sup>-1</sup> )	1.00402	0.179812

### General Power-Law

#### **MACRO : FUNCTION**

PlotPower\_Law() : Power\_Law(w,y,x)

Wave extension:     \_Power\_Law

File:

Power\_Law\_model.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

## AUTHOR/MODIFICATION

John Barker 10 FEB 1999

## APPROVED FOR DISTRIBUTION

Steve Kline 24 FEB 1999

## DESCRIPTION

Model describes a power-law including a flat background,

$$I(q) = A q^{-m} + \text{BGD}$$

with the intensity at  $q=1$  being  $A$ , decaying with power  $-m$ . The parameters  $A$ ,  $m$  and BGD can all be adjusted during fitting.

Resolution smeared version is also provided.

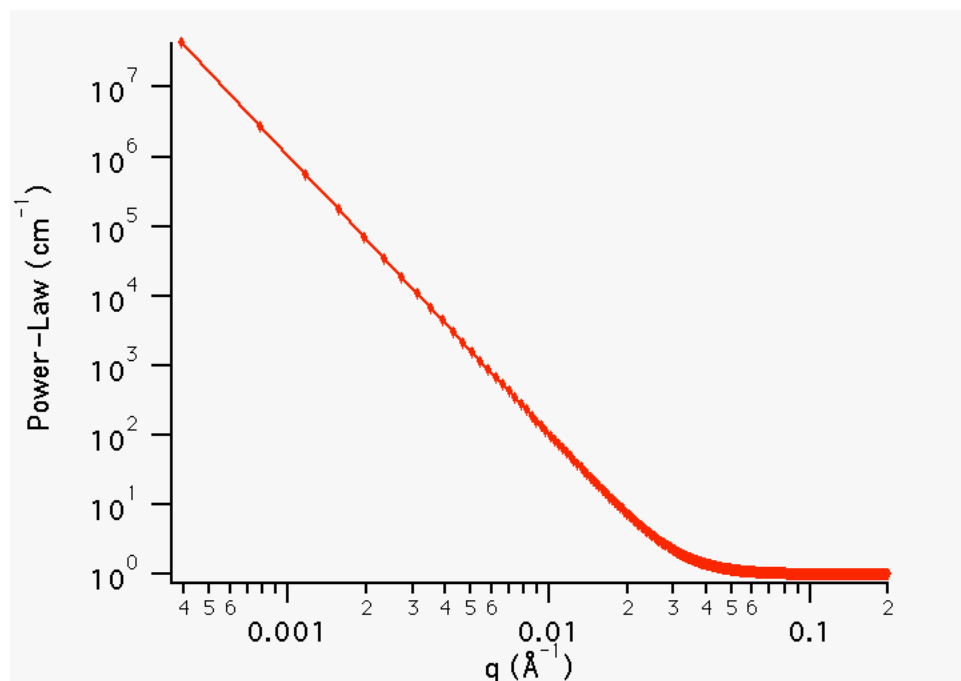
## VARIABLES

Input Variables (default values):

Point	parameters_Power_Law	coef_Power_Law
0	Coefficient, A	1e-06
1	(-)Power	4
2	Incoherent Bgd (cm <sup>-1</sup> )	1

## TEST DATASET

This example dataset is produced by the Macro PlotPower\_Law() using the default parameter values given above. The  $q$ -range has been restricted to (0.001,0.2) Å<sup>-1</sup>.



---

## **Gaussian Peak**

### **MACRO : FUNCTION**

PlotPeak\_Gauss() : Peak\_Gauss(w,y,x)

Wave extension:     \_Peak\_Gauss

File:

Peak\_Gauss\_model.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

### **AUTHOR/MODIFICATION**

John Barker   12 FEB 1999

### **APPROVED FOR DISTRIBUTION**

Steve Kline   24 FEB 1999

### **DESCRIPTION**

Model describes a Gaussian shaped peak including a flat background,

$$I(q) = I_0 \exp \left[ -1/2 \left\{ (q-q_0)/B \right\}^2 \right] + \text{BGD}$$

with the peak having height of  $I_0$  centered at  $q_{pk}$  having standard deviation of  $B$ . The fwhm is  $2.354*B$ . Parameters  $I_0$ ,  $B$ ,  $q_{pk}$ , and BGD can all be adjusted during fitting.

Resolution smeared version is also provided.

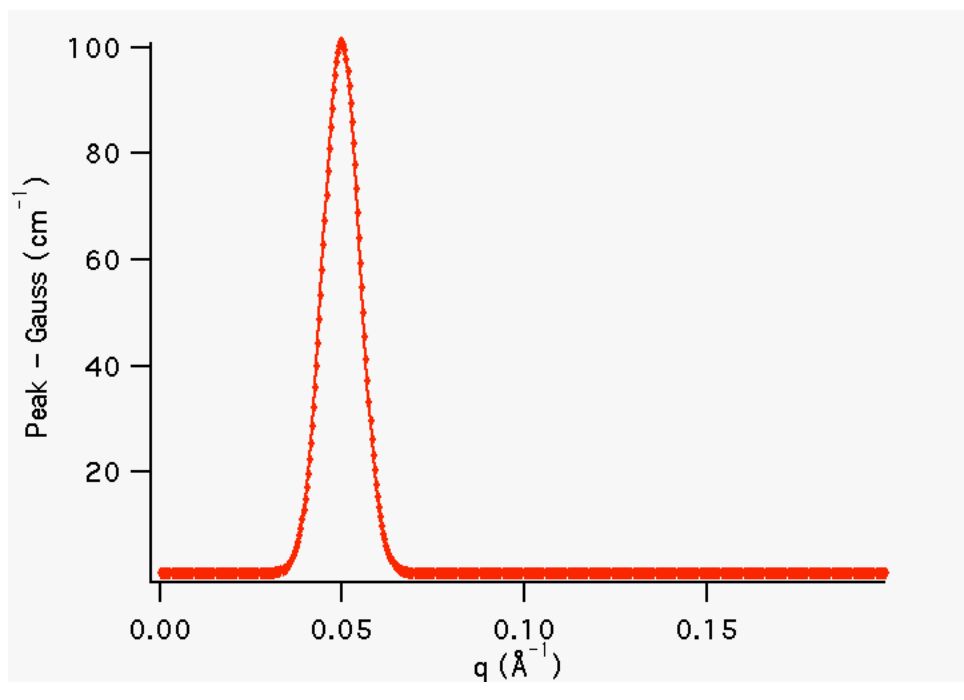
### **VARIABLES**

Input Variables (default values):

Point	parameters_Peak_Gauss	coef_Peak_Gauss
0	Scale Factor, $I_0$	100
1	Peak position ( $\text{\AA}^{-1}$ )	0.05
2	Std Dev ( $\text{\AA}^{-1}$ )	0.005
3	Incoherent Bgd ( $\text{cm}^{-1}$ )	1

### **TEST DATASET**

This example dataset is produced by the Macro PlotPeak\_Gauss() Using the default parameter values given above. The  $q$ -range has been restricted to  $(0.001,0.2) \text{ \AA}^{-1}$ .



### Lorentzian Peak

#### MACRO : FUNCTION

PlotPeak\_Lorentz() : Peak\_Lorentz(w,y,x)

Wave extension: \_Peak\_Lorentz

File:

Peak\_Lorentz\_model.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

#### AUTHOR/MODIFICATION

John Barker 10 FEB 1999

#### APPROVED FOR DISTRIBUTION

Steve Kline 24 FEB 1999

#### DESCRIPTION

Model describes a Lorentzian shaped peak including a flat background,

$$I(q) = I_0 / [ 1 + \{(q-q_0)/B\}^2 ] + \text{BGD}$$

with the peak having height of  $I_0$  centered at  $q_{pk}$  having a hwhm (half-width-half-maximum) of  $B$ . The parameters  $I_0$ ,  $B$ ,  $q_{pk}$ , and BGD can all be adjusted during fitting.

Resolution smeared version is also provided.

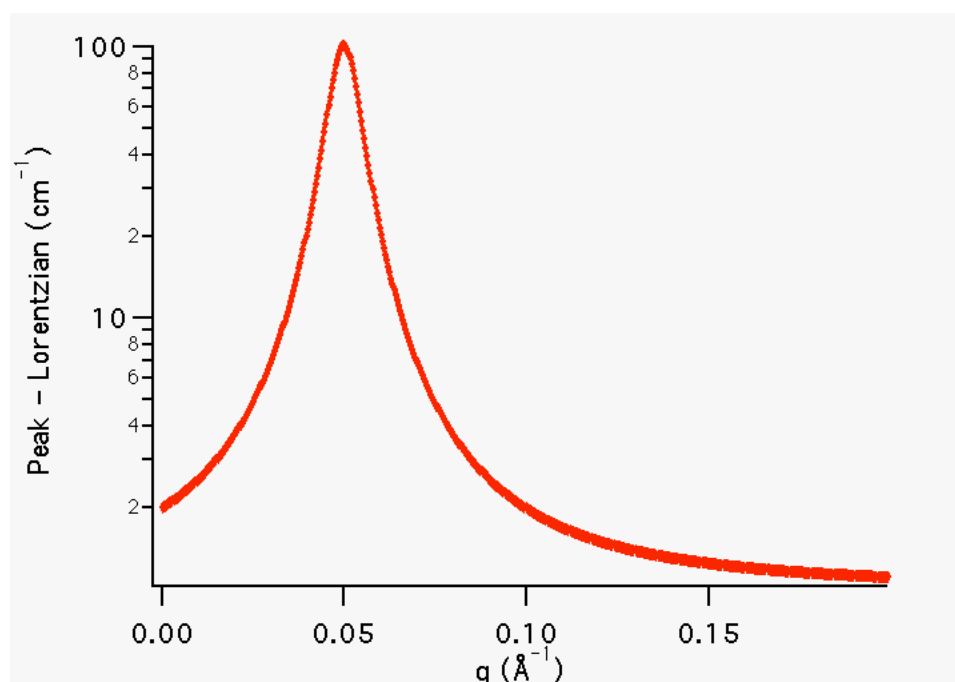
#### VARIABLES

Input Variables (default values):

Point	parameters_Peak_Lorentz	coef_Peak_Lorentz
0	Scale Factor, I0	100
1	Peak position ( $\text{\AA}^{-1}$ )	0.05
2	Peak hwhm ( $\text{\AA}^{-1}$ )	0.005
3	Incoherent Bgd (cm <sup>-1</sup> )	1

### TEST DATASET

This example dataset is produced by the Macro PlotPeak\_Lorentz() using the default parameter values given above. The q-range has been restricted to (0.001,0.2)  $\text{\AA}^{-1}$ .



### Fractal

#### MACRO : FUNCTION

PlotFractal() : Fractal(w,y,x)

Wave extension: \_fra

NumberDensity\_Fractal()

File:

Fractal.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

#### AUTHOR/MODIFICATION

Steve Kline 12 SEP 2002

## APPROVED FOR DISTRIBUTION

John Barker 17 DEC 2003

### DESCRIPTION

Calculates the scattering from fractal-like aggregates built from spherical building blocks following the Texiera reference.

A macro is provided to calculate the number density, aggregation number, and other parameters based on the volume fraction and polydisperse particle volume (weighted using the 3rd moment of the radius).

### VARIABLES

Input Variables (default values):

Point	parameters_fra	coef_fra
0	Volume Fraction (scale)	0.05
1	Block Radius (A)	5
2	fractal dimension	2
3	correlation length (A)	100
4	SLD block (A-2)	2e-06
5	SLD solvent (A-2)	6.35e-06
6	bkgd (cm <sup>-1</sup> sr <sup>-1</sup> )	0

### USAGE NOTES

The returned value is scaled to units of [cm<sup>-1</sup> sr<sup>-1</sup>], absolute scale.

The scattering intensity I(q) is calculated by

$$I(q) = P(q) S(q) + \text{bkgd}$$

where P(q) is the scattering from randomly distributed spherical "building block" particles, having radius  $R_0 = w[1]$ , volume fraction  $\phi = w[0]$ , scattering length density difference  $\Delta\rho = w[4] - w[5]$ .

$$P(q) = \phi V_p \Delta\rho^2 F(qR_0)^2$$

where  $V_p = (4/3) \pi R_0^3$  and

$$F(x) = \frac{3[\sin(x) - x \cos(x)]}{x^3}$$

The spherical building blocks aggregate to form fractal-like clusters. The clusters have a correlation length  $\xi = w[3]$  corresponding to their overall size, and self-similarity dimension  $D_f = w[2]$ . From Teixeira reference, the interference from building blocks of fractal-like cluster can be calculated from eq. 16 as

$$S(q) = 1 + \frac{\sin[(D_f - 1)\tan^{-1}(q\xi)]}{(qR_0)^{D_f}} \frac{D_f \Gamma(D_f - 1)}{\left[1 + 1/(q^2 \xi^2)\right]^{(D_f - 1)/2}}$$

The macro "NumberDensity\_Fractal" calculates the number density of building blocks  $N_0 = \phi / V_p$ , and the mean number of blocks per cluster, aggregation number  $G = S(0) = \Gamma(D+1)(\xi/R_0)^D$ , and the Guinier radius of cluster,  $R_G^2 = D(D+1)\xi^2/2$ .

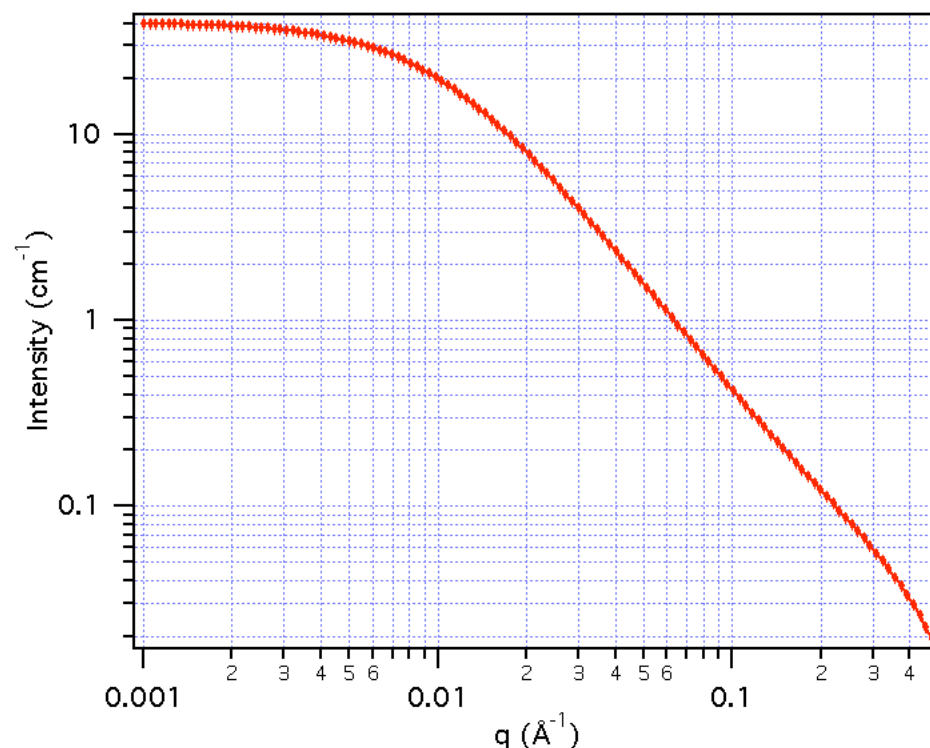
$w[0]$  (scale) and  $(w[4]-w[5])^2$  (contrast) are multiplicative factors in the model and are perfectly correlated. Only one of these parameters should be left free during model fitting.

## REFERENCE

J. Teixeira, (1988) J. Appl. Cryst., vol. 21, p781-785

## TEST DATASET

This example dataset is produced by running the Macro PlotFractal(), using 128 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.7 \text{ \AA}^{-1}$  and the above default coef\_fra values.



## Teubner-Strey

### MACRO : FUNCTION

PlotTeubnerStreyModel() : TeubnerStreyModel(w,y,x)

Wave extension: \_ts



TeubnerStreyLengths()

File:

Teubner.ipf

Requires: GaussUtils.ipf

PlotUtils.ipf

#### AUTHOR/MODIFICATION

Steve Kline 06 NOV 1998

#### APPROVED FOR DISTRIBUTION

Sungmin Choi 02 FEB 1999

#### DESCRIPTION

This function calculates the scattered intensity of a two-component system using the Teubner-Strey model. It is most applicable to microemulsions.

#### VARIABLES

Input Variables (default values):

Point	parameters_ts	coef_ts
0	scale (a2)	0.1
1	c1	-30
2	c2	5000
3	bkg	0.1

#### USAGE NOTES

The returned value is on an arbitrary scale.

the function calculated is:

$$I(q) = \frac{1}{a_2 + c_1 q^2 + c_2 q^4} + bkg$$

where the correlation length (the dispersion of d) is:

$$\xi = \left[ \frac{1}{2} \left( \frac{a_2}{c_2} \right)^{1/2} + \frac{c_1}{4c_2} \right]^{-1/2}$$

and the quasi-periodic repeat distance is:

$$\frac{d}{2\pi} = \left[ \frac{1}{2} \left( \frac{a_2}{c_2} \right)^{1/2} - \frac{c_1}{4c_2} \right]^{-1/2}$$

w[1] (= a2) acts as a scale factor, taking note that it is in the denominator and will affect the magnitude of c1 and c2.

The Macro TeubnerStreyLengths() calculates the correlation length and repeat distance based on the values in the coefficient table.

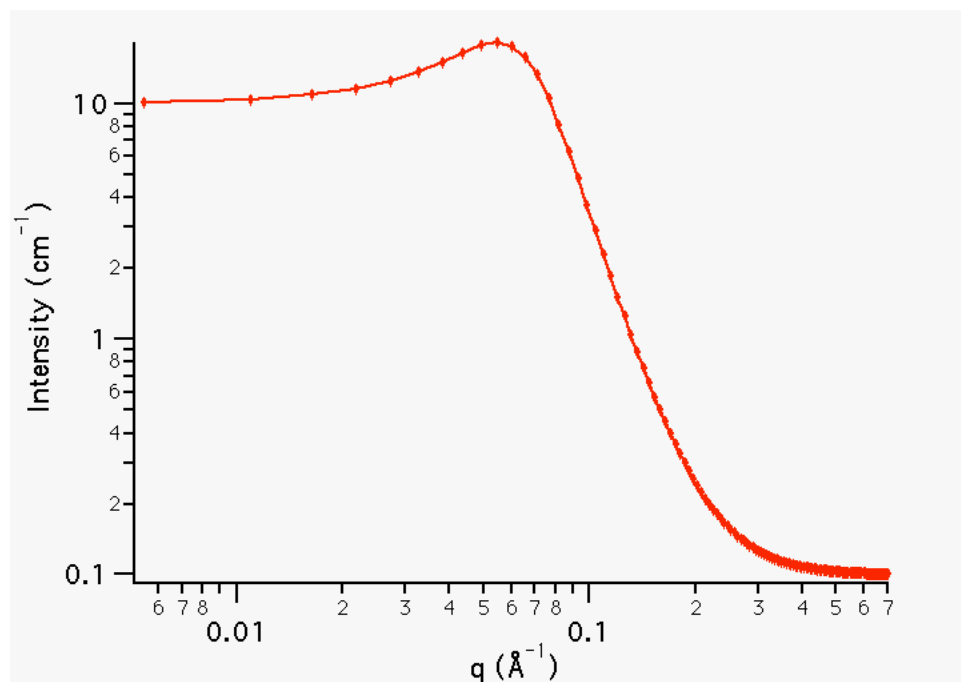
## REFERENCE

Teubner, M; Strey, R. *J. Chem. Phys.*, **1987**, *87*, 3195.

Schubert, K-V.; Strey, R.; Kline, S. R.; and E. W. Kaler *J. Chem. Phys.*, **1994**, *101*, 5343.

## TEST DATASET

This example dataset is produced by running the Macro PlotTeubnerStreyModel(), using 128 data points,  $q_{\min} = 0.001 \text{ \AA}^{-1}$ ,  $q_{\max} = 0.7 \text{ (\AA}^{-1})$  and the above default coef\_ts values.



---

## Unified Power-Law and Rg

### MACRO : FUNCTION

PlotBeau\_One() : OneLevel(w,y,x)

PlotBeau\_Two() : TwoLevel(w,y,x)

PlotBeau\_Three() : ThreeLevel(w,y,x)

PlotBeau\_Four() : FourLevel(w,y,x)

Wave extension:      \_b(N)

File:

Beaucage.ipf

Requires:

GaussUtils.ipf

PlotUtils.ipf

### AUTHOR/MODIFICATION

Steve Kline    12 SEP 2002

## APPROVED FOR DISTRIBUTION

John Barker 17 DEC 2003

## DESCRIPTION

Program incorporates the empirical multiple level unified Exponential/Power-law fit method developed by G. Beaucage. Four functions are included so that One, Two, Three, or Four levels can be used. Resolution smeared versions are provided for all models.

## VARIABLES

Input Variables (default values for two levels):

Point	parameters_b2	coef_b2
0	G1 (cm <sup>-1</sup> sr <sup>-1</sup> )	400
1	Rg1 (Å)	200
2	B1 (cm <sup>-1</sup> sr <sup>-1</sup> )	5e-06
3	Pow1	4
4	G2 (cm <sup>-1</sup> sr <sup>-1</sup> )	3
5	Rg2 (Å)	21
6	B2 (cm <sup>-1</sup> sr <sup>-1</sup> )	0.0006
7	Pow2	2
8	bkg (cm <sup>-1</sup> sr <sup>-1</sup> )	0

## USAGE NOTES

The returned value is scaled to units of [cm<sup>-1</sup> sr<sup>-1</sup>], absolute scale. The empirical expressions are able to reasonably approximate the scattering from many different types of particles, including fractal clusters, random coils (Debye equation), ellipsoidal particles, etc. The empirical fit function is

$$I(q) = Bkgd + \sum_{i=1}^N G_i \exp(-q^2 R_{g,i}^2 / 3) + \frac{B_i [erf(q R_{g,i} / \sqrt{6})]^{3P_i}}{q^{P_i}}$$

For each level, the four parameters  $G_i$ ,  $R_{g,i}$ ,  $B_i$  and  $P_i$  must be chosen.

For example, to approximate the scattering from random coils (Debye equation), set  $R_{g,i}$  as the Guinier radius,  $P_i = 2$ , and  $B_i = 2 G_i / R_{g,i}$

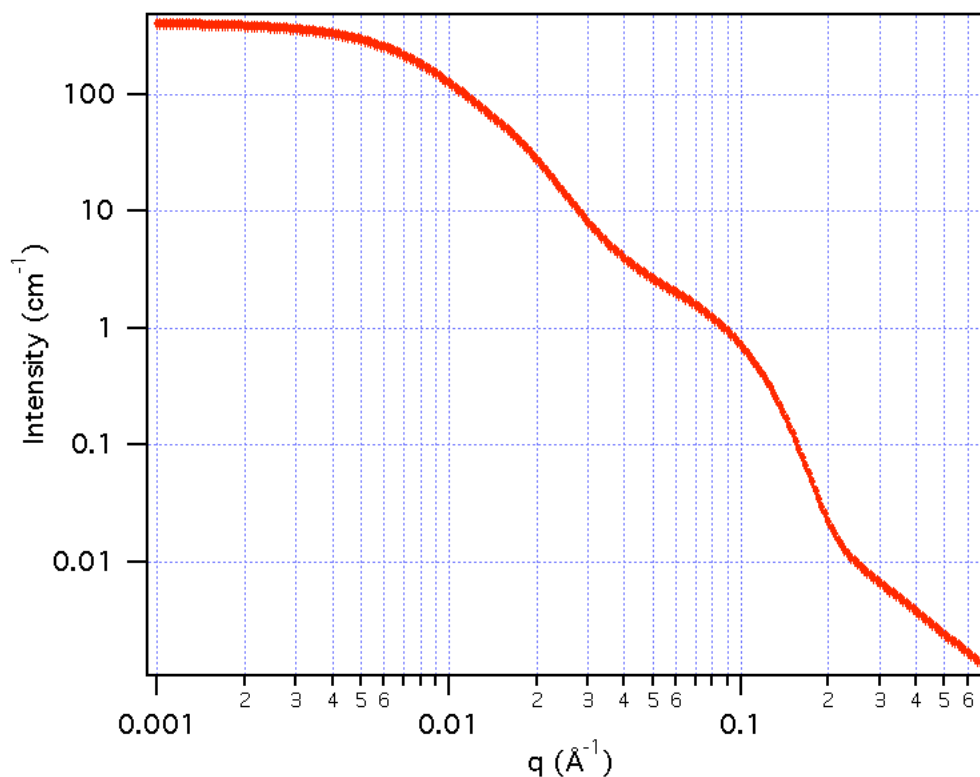
See the listed references for further information on choosing the parameters.

## REFERENCES

- G. Beaucage (1995). J. Appl. Cryst., vol. 28, p717-728.  
G. Beaucage (1996). J. Appl. Cryst., vol. 29, p134-146.

## TEST DATASET

This example dataset is produced by running the Macro PlotBeau\_two(), using 128 data points,  $q_{min} = 0.001 \text{ Å}^{-1}$ ,  $q_{max} = 0.7 \text{ Å}^{-1}$  and the above default coef\_b2 values.

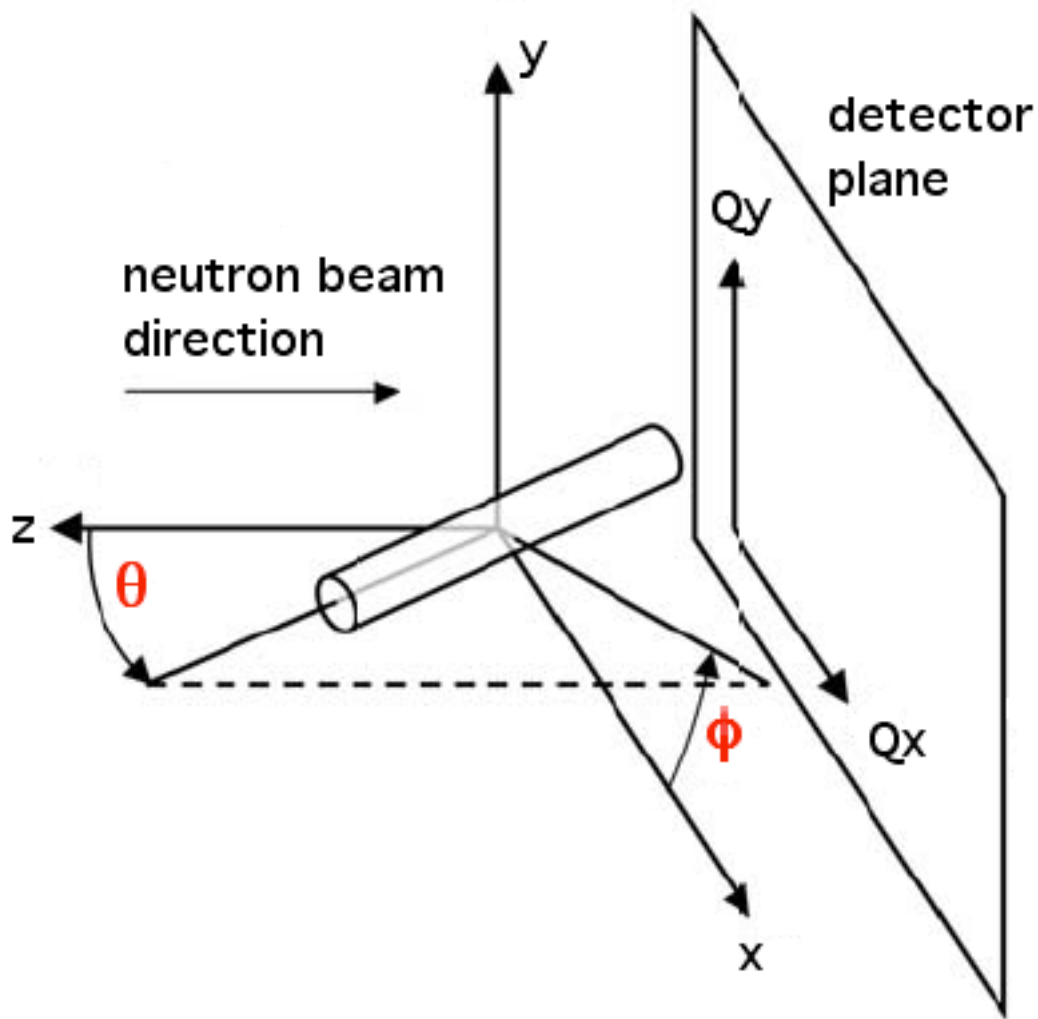


- **Anisotropic Models**

Anisotropic scattering patterns originate from the scattering of oriented materials. c-code for the 2D models has been provided as part of the DANSE project:

<<http://danse.us/trac/sans>>

For these oriented cylindrical objects, the orientation of the cylinder axis relative to the beam and detector is shown below. If a particular model has additional orientation angles they will be described as part of that model documentation. Note that theta is defined between [0,Pi] and phi is defined between [0,2Pi].



In most of the models, the following definitions apply:

- theta is defined as the angle between the axis of the cylinder and the incident beam.
- phi is defined as the angle between the axis of the cylinder and the detector plane.
- psi (in the case of an elliptical cross section) is defined as the angle between the major axis of the ellipse and the vector Q. This is related to the definition of the angle alpha, as defined below.

The scattering amplitude of many of the cylindrical models are defined in their original references in terms of an angle alpha, defined as the angle between the axis of the cylinder and Q. To convert theta and phi (above) to alpha:

$$\alpha = \cos^{-1}(\arg)$$

$$\begin{aligned} \arg = & \sin \theta \cos \phi \cdot q_x \\ & + \sin \theta \sin \phi \cdot q_y \\ & + \cos \theta \cdot q_z \end{aligned}$$

The components of Q are ( $q_x, q_y, q_z$ ). Since the SANS detector is in the xy plane,  $q_z = 0$ .

## Oriented Cylinder

### MACRO : FUNCTION

PlotCylinder2D() : Cylinder2D(w,y,x)

Wave extension: \_Cyl2D

File:

Cylinder\_2D.ipf

Requires:

PlotUtils2D.ipf

### AUTHOR/MODIFICATION

Mathieu Doucet 01 JAN 2008

### APPROVED FOR DISTRIBUTION

Steve Kline 01 FEB 2008

### DESCRIPTION

This function calculates the scattering from an oriented cylinder. The angles theta and phi define the orientation of the cylinder. A gaussian polydispersity can be added to any (or all) of the orientation angles and the radius.

### VARIABLES

Input Variables (default values):

parameters_Cyl2D	coef_Cyl2D
Scale	1
Radius	20
Length	60
SLD cylinder (A <sup>-2</sup> )	1e-06
SLD solvent	6.3e-06
Background	0
Axis Theta	1.57
Axis Phi	0
Sigma of polydisp in Radius [A]	0
Sigma of polydisp in Theta [rad]	0
Sigma of polydisp in Phi [rad]	0

### USAGE NOTES

The calculation returns the intensity, in units of [cm<sup>-1</sup>]. What is calculated is:

$$I(q) = \frac{scale}{V_{cyl}} \int d\phi \int p(\theta, \phi) F^2(q, \alpha) \sin \theta d\theta + bkg$$

The scattering amplitude of an oriented cylinder, F, is below. Alpha is the angle between the cylinder axis and Q:

$$F(q, \alpha) = 2V_{cyl} (\rho_{cyl} - \rho_{solv}) j_0(qH \cos \alpha) \frac{J_1(qr \sin \alpha)}{(qr \sin \alpha)}$$

If the polydispersity (sigma) is used for the orientation distributions,  $p(\theta, \phi)$  is a Gaussian distribution of the orientation angles. Radius distribution is an additional integration over a Gaussian distribution of radius.

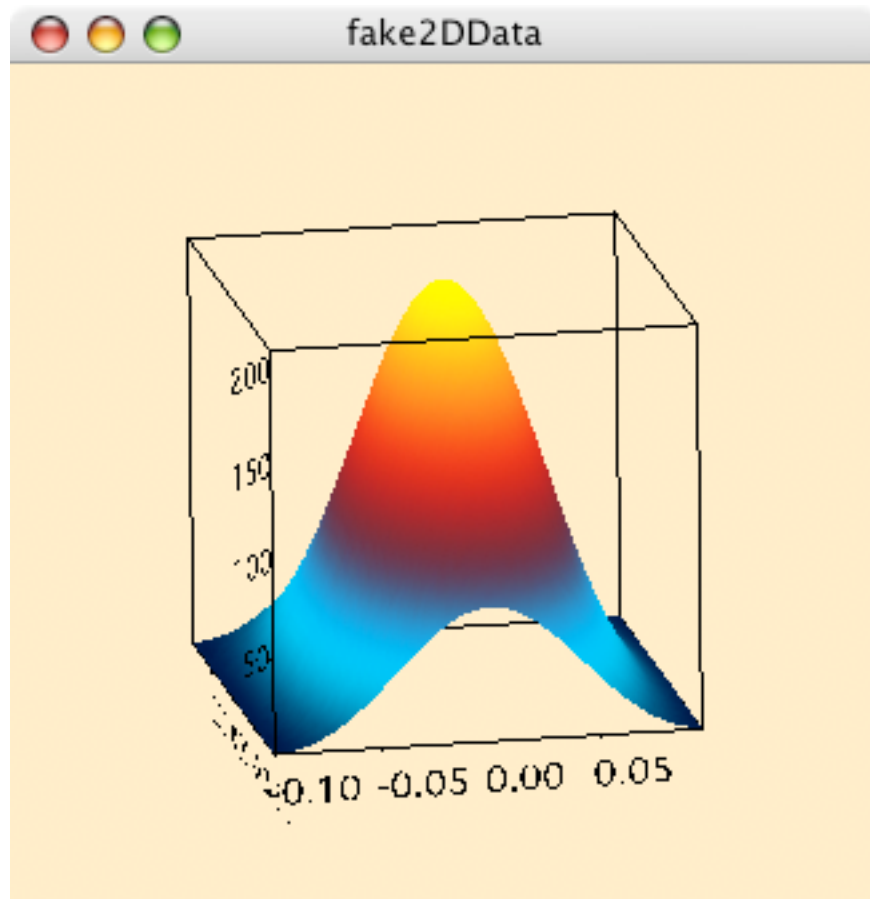
## REFERENCE

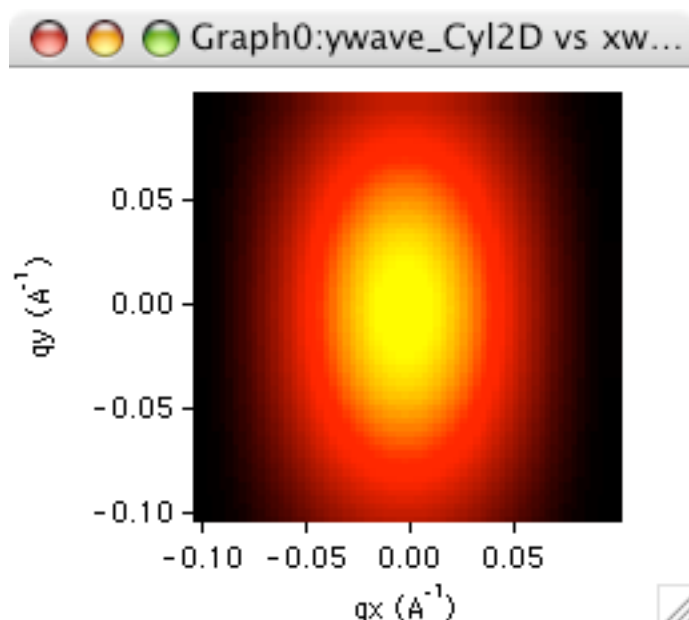
Guinier, A. and G. Fournet, "Small-Angle Scattering of X-Rays", John Wiley and Sons, New York, (1955).

## TEST DATASET

This data set is produced when plotting the 2D cylinder model using the default parameters, and a 64x64 detector with:

$$(-Q_x, Q_x)(-Q_y, Q_y) = (-0.1, 0.1)(-0.1, 0.1) [A^{-1}]$$





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### Oriented Core-Shell Cylinder

#### **MACRO : FUNCTION**

PlotCoreShellCylinder2D() : CoreShellCylinder2D(w,y,x)

Wave extension: \_CSCyl2D

File:

CoreShellCyl2D.ipf

Requires:

PlotUtils2D.ipf

#### **AUTHOR/MODIFICATION**

Mathieu Doucet 01 JAN 2008

#### **APPROVED FOR DISTRIBUTION**

Steve Kline 01 FEB 2008

#### **DESCRIPTION**

This function calculates the scattering from an oriented cylinder with a core-shell structure. The angles theta and phi define the orientation of the cylinder. A gaussian poydispersity can be added to any (or all) of the orientation angles and the radius.

#### **VARIABLES**

Input Variables (default values):



parameters_CSCyl2D	coef_CSCyl2D
Scale	1
Radius	20
Thickness	10
Length	200
Core SLD	1e-06
Shell SLD	4e-06
Solvent SLD	1e-06
Background	0
Axis Theta	1.57
Axis Phi	0
Sigma of polydisp in Radius [Angstrom]	0
Sigma of polydisp in Thickness [Angstrom]	0
Sigma of polydisp in Theta [rad]	0
Sigma of polydisp in Phi [rad]	0

## USAGE NOTES

The calculation returns the intensity, in units of [cm<sup>-1</sup>]. What is calculated is:

$$I(q) = \frac{scale}{V_{cyl}} \int d\phi \int p(\theta, \phi) F^2(q, \alpha) \sin \theta d\theta + bkg$$

The scattering amplitude of an oriented core-shell cylinder, F, is below. Alpha is the angle between the cylinder axis and Q:

$$f(q, \alpha) = 2(\rho_{core} - \rho_{shell})V_{core}j_0(qH\cos\alpha)\frac{J_1(qr\sin\alpha)}{(qr\sin\alpha)} \\ + 2(\rho_{shell} - \rho_{solvent})V_{shell}j_0[q(H+t)\cos\alpha]\frac{J_1[q(r+t)\sin\alpha]}{[q(r+t)\sin\alpha]}$$

If the polydispersity (sigma) is used for the orientation distributions, p(θ,φ) is a Gaussian distribution of the orientation angles. Radius distribution is an additional integration over a Gaussian distribution of radius.

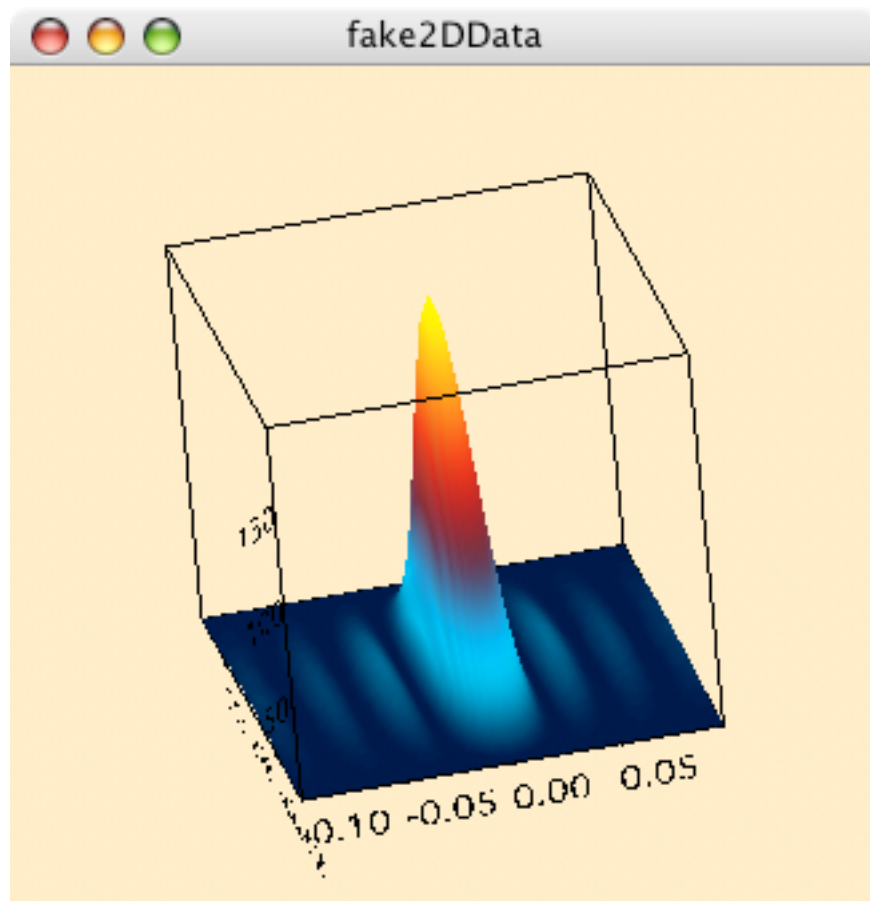
## REFERENCE

Guinier, A. and G. Fournet, "Small-Angle Scattering of X-Rays", John Wiley and Sons, New York, (1955).

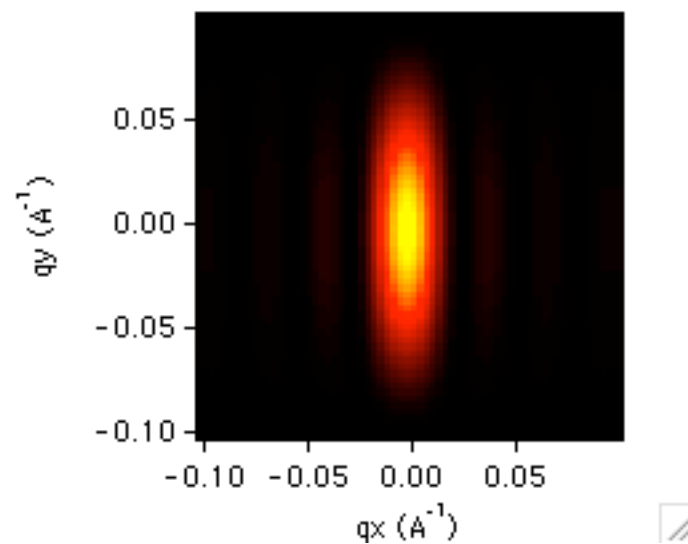
## TEST DATASET

This data set is produced when plotting the 2D core-shell cylinder model using the default parameters, and a 64x64 detector with:

$$(-Q_x, Q_x)(-Q_y, Q_y) = (-0.1, 0.1)(-0.1, 0.1) [A^{-1}]$$



Graph1:ywave\_CSCyl2D vs ...



### Oriented Elliptical Cylinder

**MACRO : FUNCTION**

PlotEllipticalCylinder2D() : EllipticalCylinder2D(w,y,x)

Wave extension: \_ElCyl2D

File:

EllipticalCylinder2D.ipf

Requires:

PlotUtils2D.ipf

## AUTHOR/MODIFICATION

Mathieu Doucet 01 JAN 2008

## APPROVED FOR DISTRIBUTION

Steve Kline 01 FEB 2008

## DESCRIPTION

This function calculates the scattering from an oriented elliptical cylinder. The angles theta and phi define the orientation of the axis of the cylinder. The angle psi is defined as the orientation of the major axis of the ellipse with respect to the vector Q. A gaussian polydispersity can be added to any (or all) of the orientation angles, and also for the minor radius and the ratio of the ellipse radii.

## VARIABLES

Input Variables (default values):

parameters_EllCyl2D	coef_EllCyl2D
Scale	1
R_minor	20
R_ratio (major/minor)	1.5
Length	400
SLD cylinder ( $A^{-2}$ )	3e-06
SLD solvent	6.3e-06
Background	0
Axis Theta	1.57
Axis Phi	0
Ellipse Psi	0
Sigma of polydisp in R_minor [Angstrom]	0
Sigma of polydisp in R_ratio	0
Sigma of polydisp in Theta [rad]	0
Sigma of polydisp in Phi [rad]	0

## USAGE NOTES

The function calculated is:

$$I(q) = \frac{scale}{V_{cyl}} \int d\psi \int d\phi \int p(\theta, \phi, \psi) F^2(q, \alpha, \psi) \sin \theta d\theta + bkg$$

with the functions:

$$F(q, \alpha, \psi) = 2 \frac{J_1(a)}{a} \cdot \frac{\sin(b)}{b}$$

$$a = q \cdot \sin(\alpha) \left[ r_{major}^2 \sin^2(\psi) + r_{minor}^2 \cos^2(\psi) \right]^{1/2}$$

$$b = q \frac{L}{2} \cos(\alpha)$$

and the angle  $\psi$  is defined as the orientation of the major axis of the ellipse with respect to the vector  $Q$ .

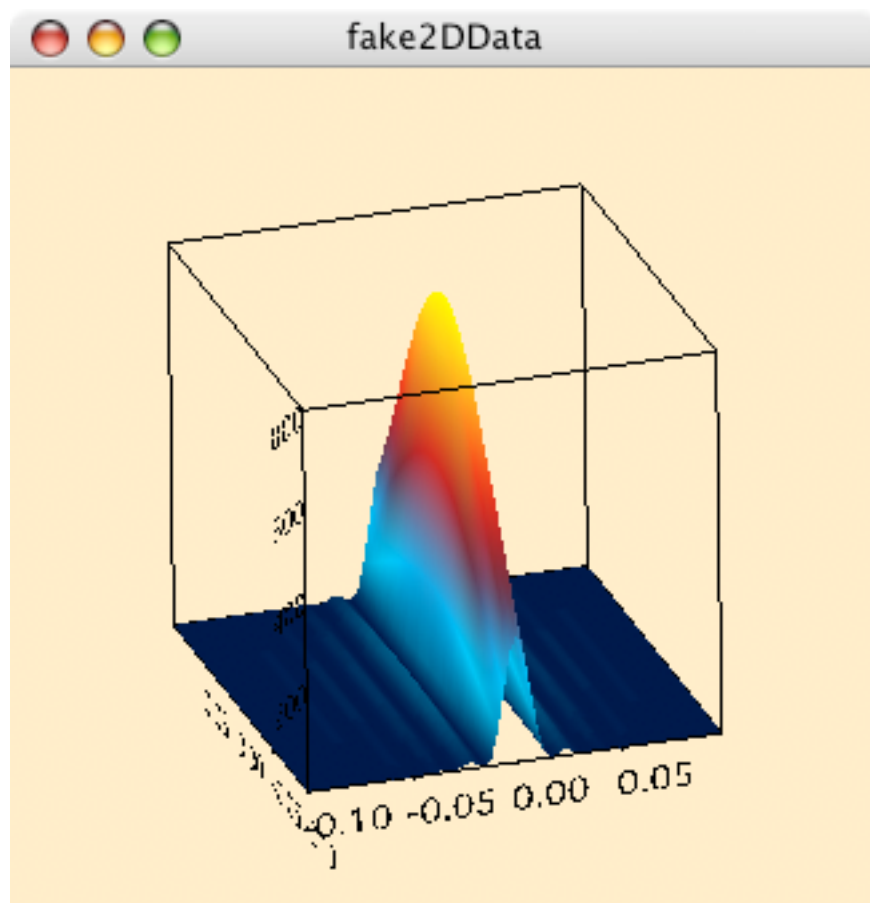
#### REFERENCE

L. A. Feigin and D. I. Svergun “Structure Analysis by Small-Angle X-Ray and Neutron Scattering”, Plenum, New York, 1987.

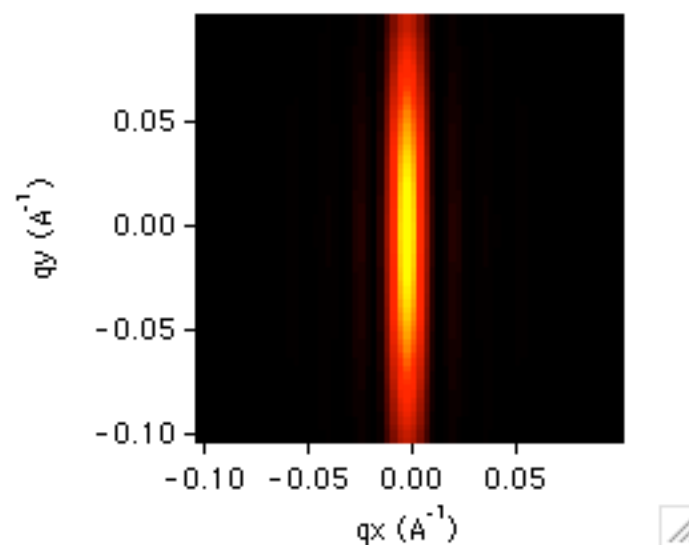
#### TEST DATASET

This data set is produced when plotting the 2D elliptical cross section cylinder model using the default parameters, and a 64x64 detector with:

$$(-Q_x, Q_x)(-Q_y, Q_y) = (-0.1, 0.1)(-0.1, 0.1) [A^{-1}]$$



Graph2:ywave\_EllCyl2D vs ...



### Oriented Ellipsoid

**MACRO : FUNCTION**

PlotEllipsoid2D() : Ellipsoid2D(w,y,x)

Wave extension:      \_Ellip2D

File:

Ellipsoid2D.ipf

Requires:

PlotUtils2D.ipf

## AUTHOR/MODIFICATION

Mathieu Doucet   01 JAN 2008

## APPROVED FOR DISTRIBUTION

Steve Kline    01 FEB 2008

## DESCRIPTION

This function calculates the scattering from an oriented ellipsoid. The angles theta and phi define the orientation of the axis of the ellipsoid. The angle theta is always taken to be the angle between the rotation axis and z. A gaussian polydispersity can be added to any (or all) of the orientation angles, and also for either radius of the ellipsoid.

## VARIABLES

Input Variables (default values):

parameters_Ellip2D	coef_Ellip2D
Scale	1
Radius_a (rotation axis)	20
Radius_b	60
SLD cylinder (A <sup>-2</sup> )	1e-06
SLD solvent	6.3e-06
Background	0
Axis Theta	1.57
Axis Phi	0
Sigma of polydisp in R_a [Angstrom]	0
Sigma of polydisp in R_b [Angstrom]	0
Sigma of polydisp in Theta [rad]	0
Sigma of polydisp in Phi [rad]	0

## USAGE NOTES

The calculation returns the intensity, in units of [cm<sup>-1</sup>]. What is calculated is:

$$I(q) = \frac{scale}{V_{cyl}} \int d\phi \int p(\theta, \phi) F^2(q, \alpha) \sin \theta d\theta + bkg$$

where the scattering amplitude is given by:

$$f(q) = \frac{3(\Delta\rho)V(\sin[qr(R_a, R_b, \alpha)] - qr \cos[qr(R_a, R_b, \alpha)])}{[qr(R_a, R_b, \alpha)]^3}$$

$$r(R_a, R_b, \alpha) = [R_b^2 \sin^2 \alpha + R_a^2 \cos^2 \alpha]^{1/2}$$

If the polydispersity (sigma) is used for the orientation distributions,  $p(\theta, \phi)$  is a Gaussian distribution of the orientation angles. Radius distribution is an additional integration over a Gaussian distribution of radius.

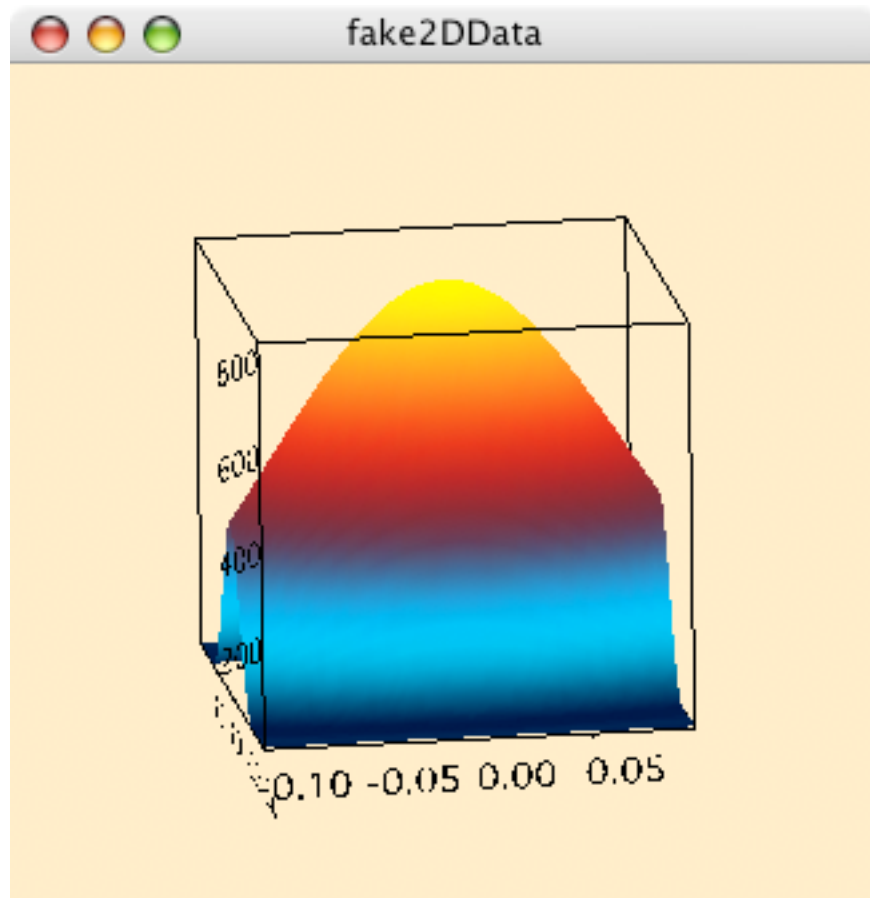
#### REFERENCE

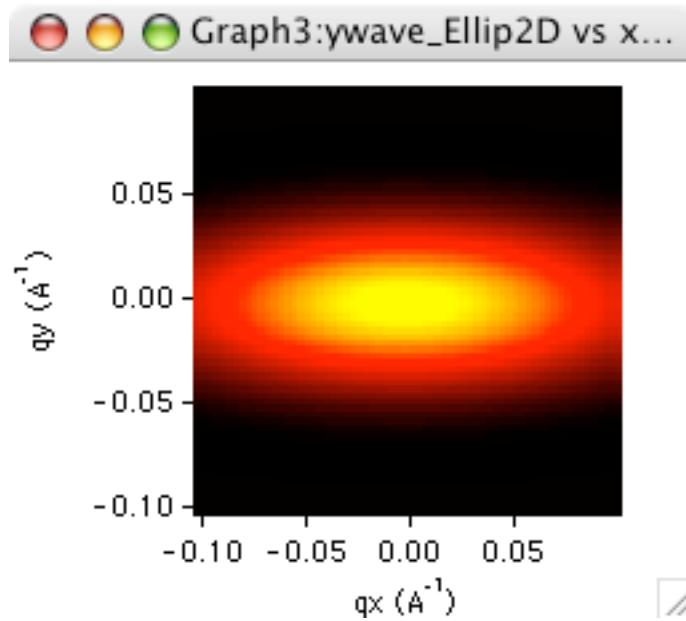
Guinier, A. and G. Fournet, "Small-Angle Scattering of X-Rays", John Wiley and Sons, New York, (1955).

#### TEST DATASET

This data set is produced when plotting the 2D ellipsoid model using the default parameters, and a 64x64 detector with:

$$(-Q_x, Q_x)(-Q_y, Q_y) = (-0.1, 0.1)(-0.1, 0.1) [A^{-1}]$$





### • How Form Factors and Structure Factors are Combined

In a colloidal dispersion, there are typically discrete particles of different atomic composition from the surrounding solvent. It is then convenient to divide the scattering volume into  $N_p$  cells, each containing one particle and structureless solvent. The scattered intensity from a collection of discrete particles can be written as:

$$\frac{d\Sigma}{d\Omega}(\vec{q}) = \frac{1}{V} \sum_{k=1}^{N_p} \langle |f_k(\vec{q})|^2 \rangle + \frac{1}{V} \left\langle \sum_{k=1}^{N_p} \sum_{\substack{j=1 \\ j \neq k}}^{N_p} f_k(\vec{q}) f_j^*(\vec{q}) e^{i\vec{q} \cdot (\vec{r}_k - \vec{r}_j)} \right\rangle \quad (1)$$

where  $\vec{r}_k$  and  $\vec{r}_j$  are the centers of mass of cells  $k$  and  $j$  respectively. The scattering amplitude is a Fourier integral of the distribution of scattering length density within each cell, but since the solvent has a constant scattering length density, only the difference in scattering length densities applies:

$$f_k(\vec{q}) = \int_{\text{particle } k} [\rho_k(\vec{r}) - \rho_{\text{soln}}] e^{i\vec{q} \cdot \vec{r}} d\vec{r} \quad (2)$$

So the scattering amplitude of a cell depends only on the scattering length density of the particle (which need not be constant) and the scattering length density of the solvent, and becomes an integral over the particle volume. For the special case of monodisperse spherical particles,  $f_k(\vec{q}) = f_j^*(\vec{q}) = f(q)$ , and Equation 1 can be factored into the form:



$$\frac{d\Sigma}{d\Omega}(\vec{q}) = n_p \left\langle |f(q)|^2 \right\rangle \left\{ 1 + \left\langle \sum_{k=1}^{N_p} \sum_{\substack{j=1 \\ j \neq k}}^{N_p} e^{i\vec{q} \cdot (\vec{r}_k - \vec{r}_j)} \right\rangle \right\} \quad (3)$$

where  $n_p$  is the number density of particles. This is compactly represented as

$$\frac{d\Sigma}{d\Omega}(\vec{q}) = n_p P(q) \cdot S(\vec{q}) \quad (4)$$

by identifying the term in the angle brackets as the form factor,  $P(q)$ , and the term in parentheses as the structure factor,  $S(q)$ .

The structure factor contains all of the information about the spatial arrangement of the particles relative to an arbitrary origin. For the case of an isotropic solution, the average can be calculated around a centrally located sphere. The orientational average can be calculated as:

$$\langle S(\vec{q}) \rangle = S(q) = 1 + 4\pi n_p \int_0^\infty [g(r) - 1] \frac{\sin qr}{qr} r^2 dr \quad (5)$$

The pair correlation function,  $g(r)$ , can be calculated using liquid state theory, and thus the structure factor can be calculated. The pair correlation function can be related to thermodynamic properties of the fluid such as pressure or compressibility. To obtain information from systems of interacting colloids, it is necessary to model the scattered intensity by calculating the form and structure factors. This is easily done for monodisperse, spherical particles. However, real colloidal dispersions are not monodisperse, and not always spherical. The following sections describe the approximations that can be used to treat the scattering from polydisperse populations, and special cases that can be treated without approximation.

The effect of interactions between particles - even excluded volume interactions - must be taken into account when interpreting the scattered intensity. For particles of known morphology, it is often desirable to determine the unknown interparticle potential. This is done by proposing an interaction potential, using statistical mechanics to calculate  $S(q)$ , and fitting the model to the data.

The interparticle potential determines the equilibrium arrangement of particles,  $g(r)$ , from which  $S(q)$  can be calculated. For a homogeneous, isotropic fluid of spheres, the Ornstein-Zernicke equation is:

$$h(r) = g(r) - 1 = c(r) + n \int c(|\vec{r} - \vec{x}|) h(x) d\vec{x} \quad (8)$$

and states that the total correlation,  $h(r)$ , between two particles is the sum of the direct correlations,  $c(r)$ , and the sum of all other correlations which are felt indirectly through all other particles. The structure factor  $S(q)$  depends directly on  $c(r)$  (compare Equations 5 and 8). Unfortunately,  $c(r)$  and  $h(r)$  are both unknown functions, and the Ornstein-Zernicke equation can only be solved if there is available an additional relation between them. This additional equation is an approximation, called a closure relation, which relates  $h(r)$  and  $c(r)$ .

The simplest of these closure relations is the Percus-Yevick closure,

$$c(r) = g(r) \left[ 1 - e^{\beta u(r)} \right] \quad (9)$$

which provides a good description of fluids with very short ranged interactions. For the simplest case of hard sphere interactions:

$$U(r) = \begin{cases} \infty & r \leq \sigma \\ 0 & r > \sigma \end{cases} \quad (10)$$

$c(r)$  is identically zero for  $r > \sigma$ . In this case an analytic solution for the structure factor can be found. Short ranged attractive interactions combined with the PY closure also yield analytical solutions for the structure factor. The first of these is the square well (SW) potential:

$$U(r) = \begin{cases} \infty & r \leq \sigma \\ -U_o & \sigma < r < \lambda\sigma \\ 0 & r > \lambda\sigma \end{cases} \quad (11)$$

The range of the square well is given by  $\lambda$ , and is typically less than 1.5. Comparison of the  $S(q)$  calculated for the square well potential to Monte Carlo data shows the calculated  $S(q)$  to be reliable for low volume fractions ( $\phi < 0.08$ ) and well depths of  $U_o < 1.5$  kT. If the attractive interactions are shorter - ranged, the sticky hard sphere potential (SHS) can be used. This is a perturbation solution of the PY closure for the case of a narrow square well of width  $\Delta$  and depth  $U_o$ . The perturbation

parameter is  $\varepsilon = \Delta/(\sigma + \Delta)$ , and must be less than 0.1. The SHS potential has the advantage that the phase diagram can be determined analytically.

The screened Coulomb interaction:

$$U(r) = \begin{cases} \infty & r \leq \sigma \\ \left( z^2 / 4\pi\epsilon\epsilon_o (1 + \kappa\sigma/2)^2 \right) \exp[-\kappa(r - \sigma)] / r & r > \sigma \end{cases} \quad (12)$$

is a good description of macroions in solution. Since the screened Coulomb repulsion is much longer ranged than hard sphere interactions, a different, more appropriate closure relation will take this into account. The mean spherical approximation (MSA) closure is:

$$c(r) = -\beta u(r) \quad (13)$$

The screened Coulomb potential can be solved for  $S(q)$  with the MSA closure using a numerical procedure. A rescaling procedure (RMSA) corrects inaccuracies that occur at low particle concentrations.

A more accurate closure relationship for charged colloids is the Rogers-Young (RY) closure. This scheme introduces an adjustable parameter,  $\alpha$ , that interpolates between the PY closure (good for short - ranged potentials) and the hypernetted chain (HNC) closure (good for longer - ranged potentials). The form of the closure is:

$$g(r) = e^{-\beta u(r)} \left\{ 1 + \frac{1}{f(r)} \left[ e^{f(r)(h(r)-c(r))} - 1 \right] \right\} \quad (14)$$

where  $f(r) = 1 - e^{-\alpha r}$ . For small values of  $r$  or  $\alpha$  the closure reduces to the PY

closure. The opposite conditions give the HNC closure. The major disadvantage of this scheme is that the integral equations must be solved numerically, and iteratively, until thermodynamic consistency is achieved, and is not (yet) implemented in these macros.

Up to this point, the discussion of form and structure factors has been limited to the simplest, but unrealistic, case of monodisperse particles. Real colloidal dispersions are polydisperse, and contain  $p$  different-sized components. To properly treat a general  $p$ -component mixture greatly complicates the analysis of SANS data, and can quickly make the problem intractable if simplifying approximations are not made. Care must be taken that any approximations are appropriate.

For a  $p$ -component mixture of spheres, the scattered intensity takes a slightly more complicated form than Equation 4:

$$\frac{d\Sigma}{d\Omega}(q) = \sum_i^p \sum_j^p (n_i n_j)^{1/2} f_i(q) f_j(q) S_{ij}(q) \quad (15)$$

but still retains the same essential features as the monodisperse form. The scattered intensity is proportional to the concentration of scatterers,  $n_i$ , the scattering amplitudes,  $f_i(q)$ , and now also the partial structure factors, defined by:

$$S_{ij}(q) = \delta_{ij} + 4\pi (n_i n_j)^{1/2} \int [g_{ij}(r) - 1] \frac{\sin qr}{qr} r^2 dr \quad (16)$$

which are the Fourier representation of the arrangement of spheres of type  $j$  around a centrally located  $i$  particle.  $\delta_{ij}$  is the Kronecker delta, and equals one if  $i = j$ , and is zero otherwise. For  $p$  components,  $p(p+1)/2$  independent partial structure factors are necessary to describe the microstructure. These are related to the partial pair correlation functions,  $g_{ij}(r)$  through the set of multicomponent Ornstein-Zernicke equations:

$$h_{ij}(r) = c_{ij}(r) + \sum_k^p n_k \int c_{ik}(|\vec{r} - \vec{x}|) h_{kj}(x) d\vec{x} \quad (17)$$

which now require a set of closure relations to relate the  $h_{ij}(r)$  to the  $c_{ij}(r)$ . This set of equations has only been solved in closed form for hard sphere mixtures. It has been solved for a binary population of spheres and for continuous Schulz-distributed spheres in the PY approximation. Interaction potentials other than hard spheres require different, more appropriate closure relations, and the set of Ornstein-Zernicke (integral) equations must be solved numerically for the partial structure factors.

For *polydisperse* spherical particles, if the particle sizes and orientations are uncorrelated, the scattered intensity can be written in a familiar form known as the "Decoupling approximation":

$$\frac{d\Sigma}{d\Omega}(q) = n_p P(q) S'(q) \quad (18)$$

with the following definitions for the average form factor:

$$P(q) = \overline{f^2(q)} \quad (19)$$

and the effective structure factor:

$$S'(q) = 1 + \left( \frac{\overline{f(q)^2}}{\overline{f^2(q)}} \right) [S(q) - 1] = 1 + \beta(q)[S(q) - 1] \quad (20)$$

where  $S(q)$  is the one component structure factor for the average radius. The horizontal bars represent an average over the size distribution. This decoupling approximation is appropriate for repulsive interaction and moderate polydispersity (<20%). For hard sphere or attractive interactions, there are significant deviations from the exact solution, especially at low  $q$ . A second, better approximation is the "Average Structure Factor" approximation, where the scattered intensity is factored into the form:

$$\frac{d\Sigma}{d\Omega}(q) = n_p \overline{f^2(q)} \cdot \overline{S}(q) \quad (21)$$

where  $\overline{S}(q)$  is the effective single component structure factor and is strictly defined by appropriate matching with the exact multicomponent expression, Equation 15. The horizontal bar over the amplitude signifies that the amplitude is first squared, then averaged over the size distribution. In the approximation,  $\overline{S}(q)$  is calculated using a monodisperse structure factor at an effective sphere diameter,  $\sigma$ , such that the approximated one-component system has the same number density  $n_p$ , and volume fraction as the polydisperse (p-component) system.

$$\sigma^3 = \frac{\sum_{i=1}^p N_i \sigma_i^3}{\sum_{i=1}^p N_i} \quad (22)$$

This approximation is superior to the decoupling approximation for hard sphere interactions and moderate polydispersities (<20%).

There are other approximations possible, but we have chosen to implement the average structure factor approximation, Equation 21, for its general accuracy and simplicity in implementation. All other approximations are still approximations, and no better or worse than this one. For spheres with excluded volume interactions (hard-sphere) and Schulz polydispersity, you can test the valid range of the approximation yourself. The PolyHSInt.ipf model is an exact, multicomponent solution for this system which you can compare to the approximate calculation for the SchulzSphere model with a hard sphere structure factor. At large polydispersities and volume fractions the approximation is clearly useless. If the particles were also non-spherical, the approximations would degrade at even lower values. Beware.

If the particles are non-spherical, but are monodisperse: the routines here take the non-spherical particle dimensions and convert them to an effective sphere diameter by equating the 2nd virial coefficient of the anisotropic particle to a sphere having the same 2nd virial coefficient. This effective sphere diameter is then used to calculate the effective structure factor. Naturally, as the particles become more anisotropic or more concentrated, the approximation becomes worse. The decoupling

approximation, Equations 18-20 could also be applied to non-spherical particles. The assumption is the same, one that the particle position is uncorrelated with its orientation. The decoupling approximation gives similar results to the average structure factor approach. It would always be preferable to have an exact technique, but there are currently none available.

Some of the model form factors do not have any  $S(q)$  combinations provided, such as:

- Cylinders with polydispersity (polydisperse AND non-spherical)
- Flexible cylinder models (can't be defined as a particle with an effective diameter)
- Parallelepiped (could use decoupling, but must first validate vs. simulations)
- Triaxial ellipsoid (could use decoupling, but must first validate vs. simulations)

When possible, the form factor models presented here have been normalized by the average particle volume,  $V_p$ , so that the scale factor is effectively ( $n V_p$  = volume fraction), which is a more natural experimental unit than number density. For dilute, polydisperse systems, the number density is correctly calculated using the average particle volume, which is not the same as the volume of the particle with the mean radius.

## References:

More details of the mathematics of scattering from colloidal solutions can be found in the following references.

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